Approximate inverse preconditioning

Some references

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- Broker, Oliver. Parallel multigrid methods using sparse approximate inverses. Thesis (Dr.sc.) Eidgenössische Technische Hochschule Zuerich (Switzerland). 2003. 169 pp
- Wang, Shun; de Sturler, Eric. Multilevel sparse approximate inverse preconditioners for adaptive mesh refinement. Linear Algebra Appl. 431 (2009), 409-426

Thomas Huckle,
Modified Sparse Approximate Inverses
http://www5.in.tum.de/wiki/index.php/MSPAI
Factorized Sparse Approximate Inverses
http://www5.in.tum.de/wiki/index.php/FSPAI
Approximate inverses: Explicit Methods

Given a sparse matrix $A = [a_{ij}] \in \mathbb{R}^{n \times n}$. Let $S$ be a sparsity pattern. We want to compute $G \in S$, such that

$$(GA)_{ij} = \delta_{ij}, \ (i, j) \in S,$$

i.e.

$$\sum_{k: (i, k) \in S} g_{ik} a_{kj} = \delta_{ij}, \ (i, j) \in S.$$ 

Some observations:

⊕ the elements in the $i$th row of $G$ can be computed independently;

⊖ even if $A$ is symmetric, $G$ is not necessarily symmetric, because $g_{ij}$ and $g_{ji}$ are, in general, not equal.

How does this work?

Choose $S$ to be the tridiagonal part of $A$, 
$S = \{(1, 1), (1, 2), \{(i, i - 1), (i, i), (i, i + 1)\}_{i=1}^{n}, (n, n - 1), (n, n)\}$. Then, when computing the $i$th row of $G$ we need only the entries of the matrix $A$, namely,

$$A^i = \begin{bmatrix}
  a_{i-1,i-1} & a_{i-1,i} & a_{i-1,i+1} \\
  a_{i,i-1} & a_{i,i} & a_{i,i+1} \\
  a_{i+1,i-1} & a_{i+1,i} & a_{i+1,i+1}
\end{bmatrix}$$

Given $A \in \mathbb{R}^{n \times n}$ and $S$ for $i=1:n$,

Extract from $A$ the small matrix $A^i$, needed to compute the entries of $G(i, :)$

Solve with $A^i$ the entries of $G(i, :)$

Store row $G(i, :)$
Example:

We want to find $G$ with the same sparsity pattern as $A$, i.e.,

$$A = \begin{bmatrix}
2 & -1 & 0 & 0 \\
-1 & 3 & -2 & 0 \\
0 & -2 & 4 & -1 \\
0 & 0 & -1 & 2
\end{bmatrix} \quad G = \begin{bmatrix}
g_{11} & g_{12} & 0 & 0 \\
g_{21} & g_{22} & g_{23} & 0 \\
0 & g_{32} & g_{33} & g_{34} \\
0 & 0 & g_{43} & g_{44}
\end{bmatrix}$$

$G(1,:) : 2g_{11} - g_{12} = 1$
$-g_{11} + 3g_{12} = 0$

$G(2,:) : 2g_{21} - g_{22} = 0$
$-g_{21} + 3g_{22} - 2g_{23} = 1$
$-2g_{22} + 4g_{23} = 0$

Example, cont.

$$A^{-1} = \frac{1}{19} \begin{bmatrix} 13 & 7 & 4 & 2 \\
7 & 14 & 8 & 4 \\
4 & 8 & 10 & 5 \\
2 & 4 & 5 & 12
\end{bmatrix}$$

$$G = \begin{bmatrix}
\frac{3}{5} & \frac{1}{5} & 0 & 0 \\
\frac{1}{3} & \frac{2}{3} & \frac{1}{3} & 0 \\
0 & \frac{1}{13} & \frac{6}{13} & \frac{2}{13} \\
0 & 0 & \frac{1}{7} & \frac{4}{7}
\end{bmatrix}$$

$$GA = \begin{bmatrix}
1 & 0 & -0.40 & 0 \\
0 & 1 & 0 & -0.33 \\
-0.31 & 0 & 1 & 0 \\
0 & -0.28 & 0 & 1
\end{bmatrix}$$
Example, cont.

Note: the second row of $G$ is the second row of the matrix

$$ B = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 3 & -2 & 0 \\ 0 & -2 & 4 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}^{-1}, \quad GB = \begin{bmatrix} 1 & 0 & -0.4 & 0 \\ 0 & 1 & 0 & 0 \\ -0.31 & 0 & 1.2308 & 0.4615 \\ 0 & -0.2857 & 0.5714 & 1.1429 \end{bmatrix}.$$  

However, if we compute $AG$ then

$$ AG = \begin{bmatrix} 0.8667 & -0.2667 & -0.3333 & 0 \\ 0.4000 & 1.1846 & 0.0769 & -0.4615 \\ -0.6667 & -0.1026 & 1.0366 & 0.3516 \\ 0 & -0.3077 & -0.1758 & 0.9121 \end{bmatrix} $$

i.e., the matrix $G$ is computed as a left-side approximate inverse of $A$ and as such is somewhat less accurate than as a right-side approximate inverse.

The drawback of the above method is that in general even if $A$ is symmetric, $G$ is not!

## Implicit Methods

Let $A$ be in a factored form.

Suppose $A = LD^{-1}U$ is a triangular matrix factorization of $A$. If $A$ is a band matrix then $L$ and $U$ are also band matrices.

Let $L = I - \tilde{L}$, $U = I - \tilde{U}$, where $\tilde{L}$ and $\tilde{U}$ are strictly lower and upper triangular matrices correspondingly.

**Lemma 1** Using the above notations it can be shown that

(i) $A^{-1} = DL^{-1} + \tilde{U}A^{-1}$,  
(ii) $A^{-1} = U^{-1}D + A^{-1}\tilde{L}$.

**Proof**

$$ A = LD^{-1}U \implies A^{-1} = U^{-1}DL^{-1} $$

$$ \implies (I - \tilde{U})A^{-1} = DL^{-1} \implies A^{-1} = DL^{-1} + \tilde{U}A^{-1}. $$

Also

$$ A^{-1}(I - \tilde{L}) = U^{-1}D \implies A^{-1} = U^{-1}D + A^{-1}\tilde{L}. $$
Algorithm to compute $A^{-1}$

for $r = n, n - 1, \ldots, 1$

$$(A^{-1})_{r,r} = D_{r,r} + \sum_{s=1}^{\min(q,n-r)} \tilde{U}_{r,r+s}(A^{-1})_{r+s,r}$$

for $k = 1, 2, \ldots, q$

$$(A^{-1})_{r-k,r} = \min(q,n-r+k) \sum_{s=1}^{\min(q,n-r+k)} \tilde{U}_{r-k,r-k+s}(A^{-1})_{r-k+s,r} \leadsto (i)$$

$$(A^{-1})_{r,r-k} = \min(q,n-r+k) \sum_{t=1}^{\min(q,n-r+k)} (A^{-1})_{r,k-t} \tilde{L}_{r-k+t,r-k} \leadsto (ii)$$

endfor

q is the bandwidth.

A drawback:

Consider an spd matrix

$\begin{bmatrix}
1 & -2 & 1 \\
-2 & 5 & -3 \\
1 & -3 & 4
\end{bmatrix}$

Then $A_{band} = \begin{bmatrix}
1 & -2 & 0 \\
-2 & 5 & -3 \\
0 & -3 & 4
\end{bmatrix}$

is indefinite.
A general framework for computing approximate inverses

Frobenius norm minimization
\[ \|A\|_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2} = \sqrt{\text{tr}(AA^T)} \]

Let a sparsity pattern \( S \) be given. Consider the functional
\[ F_W(G) = \|I - GA\|_W^2 = \text{tr}(I - GA)W(I - GA)^T, \]
where the weight matrix \( W \) is spd if \( W \equiv I \) then \( \|I - GA\|_I \) is the Frobenius norm of \( I - GA \).

Clearly \( F_W(G) \geq 0 \). If \( G = A^{-1} \) then \( F_W(G) = 0 \). Hence, we want to compute the entries of \( G \) in order to minimize \( F_W(G) \), i.e. to find \( \hat{G} \in S \), such that
\[ \|I - \hat{G}A\|_W \leq \|I - GA\|_W, \forall G \in S. \]

The following properties of \( \text{tr}(\cdot) \) will be used:
\[ \text{tr}(AB) = \text{tr}(BA), \text{tr}(A + B) = \text{tr}(A) + \text{tr}(B). \]

Minimize \( F_W \) w.r.t. \( G \), consider the entries \( g_{i,j} \) as variables. The necessary condition for a minimizing point are
\[ \frac{\partial F_W(G)}{\partial g_{ij}} = 0, (i, j) \in S. \]

From (1) and (2) we get
\[ -2(WA^T)_{ij} + 2(GAWA^T)_{ij} = 0, \text{ or} \]
\[ (GAWA^T)_{ij} = (WA^T)_{ij}, (i, j) \in S. \]

The equations (3) may or may not have a solution, depending on the particular matrix \( A \) and the choice of \( S \) and \( W \).
Choices of $W$:

**Choice 1:** Let $A$ be spd Choose $W = A^{-1}$ which is also spd

\[
(GA)_{ij} = \delta_{ij}, \quad (i, j) \in S,
\]

i.e. the formula for the explicit method can be seen as a special case of the more general framework for computing approximate inverses using weighted Frobenius norms.

**Choice 2:** Let $W = (A^T A)^{-1}$.

\[
(G)_{ij} = (A^{-1})_{ij}, \quad (i, j) \in S,
\]

which is the formula for the implicit method. In this case the entries of $G$ are the corresponding entries of the exact inverse.

---

**Improvement via diagonal compensation**

Let $A$ be symmetric and five-diagonal. Suppose we know that the two of the off-diagonals contain small entries. Such matrix appears if we solve the anisotropic problem, for instance:

\[
-\frac{\partial^2 u}{\partial x^2} - \varepsilon \frac{\partial^2 u}{\partial y^2} = f,
\]

where $\varepsilon > 0$ is small.

We choose a tridiagonal sparsity pattern $S_3$ for $G$, where the the two nonzero off-diagonals will correspond to the off-diagonals of $A$, containing bigger elements, i.e. they are not necessarily next to the main diagonal. Then we construct an approximate inverse in the following way:
Step 1: Let \( \tilde{A} \) be \( A \) with deleted small entries, i.e. \( \tilde{A} \in S_3 \).

Step 2: Compute \( \tilde{G} \): 
\[
(\tilde{G}A)_{ij} = \delta_{ij}, \quad (i, j) \in S_3.
\]

Step 3: Find \( G = \bar{G} + D \), where 
\[
\bar{G} = \frac{1}{2}(\tilde{G} + \tilde{G}^T)
\]
and \( D \) is diagonal, computed from the following imposed condition on \( G \), i.e.
\[
G A e = e,
\]
and \( e = (1, 1, \cdots, 1)^T \).

The diagonal compensation technique prescribes the spd property of \( A \).

The methods described till now do not guarantee that \( G \) will be such a matrix.
We want now to compute an spd approximate inverse of an spd matrix.

Let \( S \) be a symmetric sparsity pattern. We seek \( G \) of the form
\[
G = L_G^T L_G, \quad L_G \in S_L.
\]

Clearly \( G \) will be spd

**Theorem 1** A matrix \( G \) of the form \( G = L_G^T L_G \) which is an spd approximation of \( A^{-1} \) can be computed from the following relation:
\[
\min_{X \in S_L} \frac{1}{\pi} \frac{\frac{1}{n} \text{tr} X A X^T}{(\text{det}(X A X^T))^{\frac{1}{n}}} = \frac{1}{\pi} \frac{\frac{1}{n} \text{tr} L_G A L_G^T}{(\text{det}(L_G A L_G^T))^{\frac{1}{n}}}.
\] (4)
Proof:

$X \in S_L$ is lower triangular. Let $X = D(I - \tilde{X})$, where $\tilde{X} \in S_{\tilde{L}}$ is strictly lower triangular. Then $\tilde{X} = I - D^{-1}X$. Let denote also $D = \text{diag}(d_1, d_2, \ldots, d_n)$. Then

$$\frac{1}{n} \text{tr } XAX^T \left( \frac{\det(XAX^T)}{\det(X)^2 \det(A)} \right)^{\frac{1}{n}} = \frac{1}{n} \sum_i (XAX^T)_{ii} \left( \frac{\det(X)^2 \det(A)}{\det(XAX^T)} \right)^{\frac{1}{n}}$$

$$= \frac{1}{n} \sum_i \left( D(I - \tilde{X})A(I - \tilde{X})^T D \right)_{ii} \left( \frac{\det(X)^2 \det(A)}{\det(XAX^T)} \right)^{\frac{1}{n}} = \frac{1}{n} \sum_i d_i^2 \left( (I - \tilde{X})A(I - \tilde{X})^T \right)_{ii} \left( \frac{\det(X)^2 \det(A)}{\det(XAX^T)} \right)^{\frac{1}{n}}$$

$$= \frac{1}{n} \sum_i \alpha_i^2 \left( \frac{\prod_i (I - \tilde{X})A(I - \tilde{X})^T)_{ii}}{\prod_i \alpha_i^2} \right)^{\frac{1}{n}} \left( \frac{\det(X)^2 \det(A)}{\det(XAX^T)} \right)^{\frac{1}{n}}$$

$$= \frac{1}{n} \sum_i \alpha_i^2 \left( \frac{\prod_i (I - \tilde{X})A(I - \tilde{X})^T)_{ii}}{\prod_i \alpha_i^2} \right)^{\frac{1}{n}} \left( \frac{\det(X)^2 \det(A)}{\det(XAX^T)} \right)^{\frac{1}{n}}$$

$$= \text{Expression}_A \cdot \text{Expression}_B. \quad (5)$$

In the above notations $\alpha_i^2 = d_i^2 \left( (I - \tilde{X})A(I - \tilde{X})^T \right)_{ii}$.

$\text{Expression}_B$ does not depend on $d_i$. The problem of minimizing $\text{Expression}_B$ is a particular case of the already considered problem of minimizing the functional $F_W(G)$ with a special choice of the corresponding matrices $W = A$, $A = I$, $G = \tilde{X}$. In other words, the solution of the problem

$$\min_{\tilde{X} \in S_{\tilde{L}}} \prod_i \left( (I - \tilde{X})A(I - \tilde{X})^T \right)_{ii} = \min_{\tilde{X} \in S_{\tilde{L}}} \text{tr } (I - \tilde{X})A(I - \tilde{X})^T \quad (6)$$

will be also the solution of minimizing $\text{Expression}_B$.

Further, $\text{Expression}_A \geq 1$, $\forall \alpha$, being the ratio of the arithmetic and geometric mean, and takes the value 1 when $\alpha_i^2 = 1$. 

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Further, $\text{Expression}_A \geq 1$, $\forall \alpha$, being the ratio of the arithmetic and geometric mean, and takes the value 1 when $\alpha_i^2 = 1$. 

In the above notations $\alpha_i^2 = d_i^2 \left( (I - \tilde{X})A(I - \tilde{X})^T \right)_{ii}$.
Thus, we minimize Expression $A$ computing

$$d_i = \frac{1}{\left((I - \tilde{X})A(I - \tilde{X})^T\right)_{ii}^{\frac{1}{2}}}.$$  \hfill (7)

Let $\tilde{L}_G$ be the solution of (7). Note that it is strictly lower triangular. Let the entries $d_i$ of $D$ are computed from the relations (7), where instead of $\tilde{X} \tilde{L}_G$ is used. Then the matrix $L_G^T L_G$, where $L_G = D(I - \tilde{L}_G)$, will be the searched approximation of $A^{-1}$:

- $(L_G^T L_G)_{ii} = 1$ by construction;
- The equality (4) gives a measure of the quality of the approximate inverse constructed (the K-condition number (Igor Kaporin)).

Let $A = \text{tridiag}(-1, 4, -1)$. Find $L_G^T L_G$ - an approximate inverse of $A$, where $L_G$ is bidiagonal. Thus, $S_{\tilde{L}} = \{(i - 1, i)\}_{i=2}^n$.

First we compute a strictly lower bidiagonal matrix $\tilde{L}$ from the condition

$$(\tilde{L}A)_{i,j} = (A)_{i,j}, \ i,j \in S_{\tilde{L}},$$

which gives us

$$\tilde{L} = \begin{bmatrix}
0 & 0 & \frac{1}{4} & \frac{1}{4} & 0 \\
\frac{1}{4} & 0 & \frac{1}{4} & 0 & \ddots \\
\frac{1}{4} & 0 & \ddots & \ddots & \frac{1}{4} \\
\frac{1}{4} & 0 & \ddots & \ddots & \ddots \\
\frac{1}{4} & 0 & \ddots & \ddots & \ddots
\end{bmatrix}.$$

Then $d_i$ are found to be

$$d_1 = \frac{1}{2}, \ d_i = \frac{2}{\sqrt{15}}, \ i = 1, 2, \ldots, n.$$
Extensions

When minimizing $\|I - AG\|_F$, minimize the 2-norm of each column separately, $\|e_k - Ag_k\|_F, k = 1, \cdots, n$

- use adaptive $S$ (much more expensive)
- used the sparsity pattern of powers of $A$
- Modified SPAI: combines
  - Frobenius norm minimization
  - MILU
  - vector probing
Consider the formulation:
\[
\min_G \|CG - B\|_F = \min_G \left\| \begin{bmatrix} C & B_0 \\ \rho e^T C & \rho e^T B_0 \end{bmatrix} \right\|_F
\]
\(\rho = 0, C_0 = A, B_0 = I\) - the original form
\(C_0 = I, B_0 = A\) - explicit approximation of \(A\)
\(\rho = [1, 1, \ldots, 1]\) - MILU
Increase existing approximations:
\[
\min_U \left\| \begin{bmatrix} L & A \\ \rho e^T L & \rho e^T A \end{bmatrix} \right\|_F
\]
Finite element setting:
\[
A = \sum_{k=1}^M R_k^T A_k R_k,
\]
with \(R_k\) being the Boolean matrices which prescribe the local-to-global correspondence of the numbered degrees of freedom.
Is this of interest?
\[
B^{-1} = \sum_{k=1}^M R_k^T A_k^{-1} R_k.
\]
\(B^{-1}\) and \(A^{-1}\) are spectrally equivalent, namely, for some \(0 < \alpha_1 < \alpha_2\) there holds
\[
\alpha_1 A_{11}^{-1} \leq B_{11}^{-1} \leq \alpha_2 A_{11}^{-1}.
\]
Finite element setting:

Consider spd matrices.

\[
\min_M (\lambda_{\min}(A_k)) \leq \lambda(A) \leq p \max_M (\lambda_{\max}(A_k)),
\]

where \( p \) is the maximum degree of the graph representing the discretization mesh. Similarly, there holds

\[
\min_M (\lambda_{\min}(A_k)^{-1}) \leq \lambda(B^{-1}) \leq p \max_M (\lambda_{\max}(A_k)^{-1}).
\]

Then we obtain

\[
\min(M \lambda_{\min}(A_k)) \leq x^T B^{-1} x \leq \max(M \lambda_{\max}(A_k))
\]

\[
\min(M \lambda_{\min}(A_k)) \leq \frac{x^T A^{-1} x}{\min(M \lambda_{\min}(A_k))} \leq \max(M \lambda_{\max}(A_k)).
\]

Thus, the spectral equivalence constants do not depend on the mesh parameter \( h \) but they are in general robust neither with respect to problem and mesh-anisotropies, nor to jumps in the problem coefficients as the eigenvalues of \( A_k \) depend on those.
The matrix itself ($\text{mesh}(A)$)

The approximate inverse ($\text{mesh}(A^{-1})$)
The exact inverse matrix \( \text{mesh}\left(\text{inv}(A)\right) \)

The difference \( \text{mesh}\left(\text{inv}(A) - AI\right) \)
FEM-SPAI: Scalability figures: Constant problem size

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Problem size: 787456
Solution method: PCG
Relative stopping criterion: \(< 10^{-6}\)
FEM-SPAI: Scalability figures: Constant load per processor

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Local number of degrees of freedom: 197129
Solution method: \textit{PCG}
Relative stopping criterium: $< 10^{-6}$