D-iteration method or how to improve Gauss-Seidel method

Dohy Hong
Alcatel-Lucent Bell Labs
Route de Villejust
91620 Nozay, France
dohy.hong@alcatel-lucent.com

ABSTRACT
The aim of this paper is to present the recently proposed fluid diffusion based algorithm in the general context of the matrix inversion problem associated to the Gauss-Seidel method. We explain the simple intuitions that are behind this diffusion method and how it can outperform existing methods. Then we present some theoretical problems that are associated to this representation as open research problems. We also illustrate some connected problems such as the graph transformation and the PageRank problem.

Categories and Subject Descriptors
G.1.3 [Mathematics of Computing]: Numerical Analysis—Numerical Linear Algebra; G.2.2 [Discrete Mathematics]: Graph Theory—Graph algorithms

General Terms
Algorithms, Performance

Keywords
Computation, Iteration, Fixed point, Gauss-Seidel, Eigenvector.

1. INTRODUCTION
In this paper, we revisit the very well known linear algebra equation problem:

\[ A.X = B \]

where \( A \) is a square matrix of size \( N \times N \) and \( B \) a vector of size \( N \) with unknown \( X \). There are many known approaches to solve such an equation: Gaussian elimination, Jacobi iteration, Gauss-Seidel iteration, SOR (successive over-relaxation), Richardson, Krylov, Gradient method, etc cf. [1][2][3].

In this paper, we propose a new iteration algorithm based on the decomposition of matrix-vector product as a fluid diffusion model. This algorithm has been initially proposed in the context of PageRank problem [5]. The fluid diffusion idea was first introduced in [1].

1.1 Different iterative methods
The solution of \( A.X = B \) can be solved in particular with iterative methods such as Jacobi or Gauss-Seidel iterations, when \( A \) satisfies certain conditions (e.g. strictly diagonally dominant or symmetric and positive definite).

We recall the Jacobi iteration defined by the formula:

\[ x_i^{(k+1)} = \frac{1}{a_{ii}} \left( b_i - \sum_{j \neq i} a_{ij} x_j^{(k)} \right), i = 1, 2, \ldots, N. \]

and the Gauss-Seidel iteration:

\[ x_i^{(k+1)} = \frac{1}{a_{ii}} \left( b_i - \sum_{j > i} a_{ij} x_j^{(k)} - \sum_{j < i} a_{ij} x_j^{(k+1)} \right), i = 1, 2, \ldots, N. \]

Both iterations are element-wise formula. The main difference is that in Jacobi iteration the computation of \( X^{(k+1)} \) uses only the elements of \( X^{(k)} \) (similar to power iteration method in eigenvector problem) whereas in Gauss-Seidel iteration the computation of \( x_i^{(k+1)} \) exploits the elements of \( x_j^{(k+1)} \) that have already been computed for \( j < i \). And this is the main reason which explains why the Gauss-Seidel method is generally more efficient than Jacobi iteration (when the convergence condition is satisfied). However, unlike the Jacobi method, the Gauss-Seidel method is not adapted for a distributed computation, because the values at each iteration are dependent on the order of the choice on \( i \) and there is not much freedom.

The approach proposed here, which we will call D-iteration (as Diffusion based iteration), is a new improvement idea that exploits the progressive update at the vector entry level as Gauss-Seidel with the advantage of being iteration order independent which makes it a very interesting candidate for an asynchronous distributed computation.

1.2 Collection vs Diffusion methods
For the sake of simplicity and intuitive explanation, we associate the Gauss-Seidel method to an operation of collection (one entry of vector is updated based on the previous vector based on the incoming links).

\[ \text{Collection} \]

\[ \text{Diffusion} \]

Figure 1: Intuition: collection vs diffusion.

Our approach consists in an operation of diffusion (the
fluid diffusion from one entry of the vector consists in updating all children nodes following the outgoing links) (cf. Figure 1). When the iteration is based on vector level update (such as Jacobi iteration or Power iteration), the collection or diffusion approaches become equivalent (full cycle operations on all entry of the vector).

Figure 2: Intuition: matrix product decomposition.

Somewhat, those two types of operations can be seen as dual operations, but with different consequences. With the diffusion approach, we have a very powerful result on the convergence (monotone with an explicit information on the distance to the limit, cf. [5]) and more importantly on the independence in the order of vector entries on which the diffusions are applied.

Figure 3: Intuitive comparison.

From the intuitive point of view, D-iteration can outperform the Gauss-Seidel approach by the appropriate optimized choice of the sequence of the vector coordinates for the diffusion and by its distributive computation.

2. D-ALGORITHM

2.1 Notations

We reuse here the notation introduced in [5]: \( P \) is a square matrix of size \( N \times N \) such that each column sums up to less than one (stochastic or sub-stochastic matrix).

The D-algorithm has been initially defined in the PageRank eigenvector context associated to the iteration of an equation of the form:

\[
X_{n+1} = AX_n
\]

where \( A \) is a matrix of size \( N \times N \) which can be explicitly decomposed as:

\[
A = dP + (1-d)V1^T
\]

where \( V \) is a normalized vector of size \( N \) (in the context of PageRank, the vector \( V \) is a personalized initial condition cf. [7]) and \( 1 \) is the column vector with all components equal to one. So we have:

\[
X_{n+1} = dPX_n + (1-d)V.
\]

The idea of the fluid diffusion is associated to the computation of the power series:

\[
S_\infty = (1-d) \sum_{k=0}^{\infty} d^k P^k V = (1-d)(I_d - dP)^{-1}V = X
\]

where \( I_d \) is the identity matrix and which defines the limit of the equation (3).

We define \( J_k \) a matrix with all entries equal to zero except for the \( k \)-th diagonal term: \((J_k)_{kk} = 1\).

In the following, we assume given a deterministic or random sequence \( I = \{i_1, i_2, ..., i_n, ...\} \) with \( i_n \in \{1, ..., N\} \). We only require that the number of occurrence of each value \( k \in \{1, ..., N\} \) in \( I \) to be infinity.

We recall the definition of the two vectors used in D-iteration: the fluid vector \( F \) associated to \( I \) by:

\[
F_0 = (1-d)V
\]

\[
F_n = dPJ_n F_{n-1} + \sum_{k \neq i_n} J_k F_{n-1}
\]

\[
= (I_d - J_{i_n} + dP J_{i_n})F_{n-1}.
\]

And the history vector \( H \) by:

\[
H_n = \sum_{k=1}^{n} J_{i_k} F_{k-1}.
\]

It is shown in [5] that \( H_n \) satisfies the iterative equation:

\[
H_n = (I_d - J_{i_n} (I_d - dP))H_{n-1} + J_{i_n} (1-d) V
\]

and that \( H_n \) converges to the limit \( X \) whatever the choice of the sequence \( I \). The \( L_1 \) norm of \( F_n \) gives the exact distance to the limit, if the matrix \( P \) has no zero column vector (otherwise, it defines an upper bound of the distance).

2.2 Pseudo-code

We recall here the pseudo-code presented in [5]:

**Initialization:**

\[
H[i] := 0;
F[i] := F_0[i];
\]

\[
r := |F|;
\]

**Iteration:**

\[
k := 1;
\]

While ( \( r/(1-d) > \text{Target\_Error} \) )

Choose \( i_k \);

\[
\text{sent} := F[i_k];
\]

\[
H[i_k] += \text{sent};
F[i_k] := 0;
\]

If ( \( i_k \) has no child )

\[
r -= F[i_k] * (1-d);
\]

else

For all child node \( j \) of \( i_k \):

\[
F[j] += \text{sent} * \text{p}(j,i_k) * d;
\]

\[
r -= F[i_k] * (1-d);
\]

\[
k++;
\]
$H_0$ is initialized to 0 and $F_0$ to $(1-d)V$ when associated to the equation $\mathbf{3}$ (the constant vector). In the case of the linear equation $A.X = B$, $F_0$ is initialized to $B$ or $cB$ (cf. Section 2.4).

2.3 Convergence condition

Here we only discuss the sufficient convergence condition based on the diagonally dominant matrix.

2.3.1 Diagonal dominant

We recall that $A$ is strictly diagonally dominant (by columns) if:

$$|a_{ii}| > \sum_{j \not= i} |a_{ji}|, \text{for all } i.$$ 

For the Gauss-Seidel iteration, it is more natural to consider the row version of the strictly diagonally dominant condition, whereas for the diffusion point of view the column version is natural. However, as for the Gauss-Seidel convergence condition, both conditions guarantee the convergence of the D-iteration.

2.3.2 Fluid diffusion reduction

We say that $A$ satisfies the fluid diffusion reduction condition if:

$$\sum_{j=1}^{N} |a_{ji}| < 1, \text{for all } i.$$ 

A strictly sub-stochastic matrix (for all columns) is a specific case satisfying such a condition. This can be seen as a specific case of contractive matrix.

Here, we could also define the row version for the diffusion reduction.

Finally, as for the convergence condition of the Gauss-Seidel iteration, the D-iteration converges if for at least one column, we have the fluid diffusion reduction and for the other we have the equality $\sum_{j=1}^{N} |a_{ji}| = 1$ when $A$ is irreducible.

2.4 Connection to the linear equation $A.X = B$

We can rewrite the equation $A.X = B$ as:

$$X = (I_d - A).X + B.$$ 

Then, if $X$ is a normalized probability vector $\sum_{i=1}^{N} x_i = 1$, we can replace $B$ by $B.1^T.X$ to get:

$$X = P.X$$

with $P = (I_d - A) + B.1^T$. We can recognize here the specific case of the PageRank equation $\mathbf{5}$ for which $B = (1-d)V$ and $I_d - A = dP$ (\mathbf{4}).

Equivalently, from an affine iteration equation $X_{n+1} = P.X_n + B$, we can associate to its limit $X$ a linear equation $A.X = B$ with $A = I_d - P$.

Now we can rewrite $A.X = B$ as $cA.X = cB$ for any $c > 0$ and

$$X = (I_d - cA).X + cB.$$ 

We define $P(c) = (I_d - cA)$. Without any loss of generality, we can assume that all diagonal terms of $A$ are positive (otherwise we can multiply the corresponding line vector of $A$ and the corresponding $B$’s entry by -1).

**Theorem 1.** $A$ is strictly diagonally dominant (per column), if and only if for all $c < \frac{1}{\max_{i,j: a_{ij} \neq 0} |a_{ij}|}$ (and $c > 0$), $P(c)$ satisfies the fluid diffusion reduction condition.

**Proof.** When $A$ is strictly diagonally dominant (per column), then for all $c < \frac{1}{\max_{i,j: a_{ij} \neq 0} |a_{ij}|}$:

$$\sum_i |(P(c))_{ij}| = 1 - c|a_{ii}| + \sum_{j \not= i} c|a_{ji}| < 1.$$ 

The last inequality uses exactly the strictly diagonally dominant property. Therefore this defines a necessary and sufficient condition.

2.5 Connection to the general eigenvector problem: $X = P.X$

Here we assume that we want to solve the eigenvector equation $X = P.X$ and that we have a square matrix $R$ such that $R.X = V$. Then we have:

$$X = (P - R).X + V.$$ 

If the spectral radius of $P - R$ is strictly less than 1, we can apply the D-iteration to compute $X$.

If $P$ is a transition matrix and if we are looking for a probability vector $X = P.X$, we have in particular $R = (\alpha/N)J$ where $J$ is a matrix with all entries equal to 1 and $\alpha > 0$ (in case of PageRank equation, we use $R = ((1-d)/N)J$).

We illustrate this through a simple example: take the transition matrix $P = \begin{pmatrix} 0.5 & 1 \\ 0.5 & 0 \end{pmatrix}$ and we want to find the stationary probability $X = P.X$.

![Figure 4: Example: solving $X = P.X$](image)
have:
\[ \sum_i |p_{ij} - \alpha/N| = \sum_i |p_{ij} - \alpha/N|1_{p_{ij} > \alpha/N} + \sum_i |p_{ij} - \alpha/N|1_{p_{ij} < \alpha/N}. \]

And we have \( \sum_i p_{ij} = 1 \), therefore \( \sum_i (p_{ij} - \alpha/N) = 1 - \alpha \) and
\[ \sum_i |p_{ij} - \alpha/N|1_{p_{ij} > \alpha/N} = 1 - \alpha + \sum_i |p_{ij} - \alpha/N|1_{p_{ij} < \alpha/N}. \]

Hence
\[ \sum_i |p_{ij} - \alpha/N| = 2 \times \sum_i |p_{ij} - \alpha/N|1_{p_{ij} < \alpha/N} + 1 - \alpha \]
\[ \leq 2 \times \sum_i \alpha/N1_{p_{ij} < \alpha/N} + 1 - \alpha \]
\[ \leq 2 \times (N - N^+(i, \alpha))\alpha/N + 1 - \alpha \]
\[ < 1. \]

Remark 1. If \( P \) is irreducible, it is sufficient to have \( N^+(i, \alpha) \geq N/2 \) and for at least one column, a strict inequality.

Remark 2. Obviously, the practical condition of the above theorem is to have \( N^+(i, \alpha) = |\{j : p_{ij} > 0\}| < N/2 \) for all \( i \).

3. LINK ELIMINATION

The fluid diffusion model can be in the general case described by the matrix \( P \) associated with a weighted graph \( (p_{ij} \text{ is the weight of the edge from } j \text{ to } i) \) and the initial condition \( F_0 \). So if there is a unique limit \( X \) from this setting, we can set \( X = X(P, F_0) \), which means that \( X \) is the limit of the D-iteration applied on \( (P, F_0) \).

3.1 Diagonal link elimination

Thanks to the freedom on the sequence \( I \), we have the following result:

Theorem 3. We have the equality (suppression of all diagonal term \( p_{ii} \) such that \( p_{ii} \neq 1 \); anyway if \( p_{ii} \geq 1 \), the D-iteration diverges): \( X(P, F_0) = X(P', F'_0) \) where

• \( (F'_0)_i = (F_0)_i \times \frac{1}{1-p_{ii}} \) and \( (P')_{ii} = 0; \)
• and if \( i \neq j \), \( (P')_{ij} = p_{ij} \times \frac{1}{1-p_{ii}} \).

![Figure 5: Diagonal elimination.](image)

Proof. The result is straightforward noticing that the self-diffusion \( p_{ii} \) is to be applied to \( (F_0)_i \) and to all fluids coming from incoming links. Such an operation is equivalent to the product by \( \frac{1}{1-p_{ii}} \).

Figure 6 illustrates a simple example: the suppression of the link \( p_{11} = 0.75 \) implies a multiplication by \( 1/(1-0.75) = 4 \) of \( (F_0)_1 \) and \( p_{21} = 0 \), so that we have in this case:
\[ X([0.75, 0.5, 0.1, 0]; [1, 1]) = X([0.5, 0.4]; [4, 1]) \]

![Figure 6: Diagonal elimination: example.](image)

3.2 Non-diagonal link elimination

We can extend the above operation in a general case when any link \( p_{ij} \) is suppressed (but after the diagonal suppression).

Theorem 4. We assume that \( p_{ij'} = 0 \). Then, we have the equality (elimination of the link \( p_{ij'} \) from \( i' \) to \( j' \), \( j' \neq i' \): \( X(P, F_0) = X(P', F'_0) \) where

• for \( j \neq j' \), \( (F'_0)_{ij} = (F_0)_{ij}; \)
• \( (F'_0)_{ij'} = (F_0)_{ij'} \times (F_0)_{ij} \);
• and \( (P')_{ij} = p_{ij} \) except for all \( i \) an origin node of an incoming link to \( i' \), \( (P')_{ij'} = p_{ij'} \times p_{ij'} \).

Proof. The result is straightforward noticing that the elimination of the link from \( i' \) to \( j' \) affects only the fluid that goes to \( j' \) with the D-iteration: therefore we need to push to \( j' \) the initial fluid \( (F_0)_{ij} \) and add a new link (or modify the weight of the existing one) from all origin nodes of an incoming link to \( i' \) which would replace the fluid going from \( i \) to \( j' \) though \( i' \).

![Figure 7: Link \( p_{ij'} \) elimination.](image)

Figure 8 illustrates a simple example: the suppression of the link \( p_{21} = 0.5 \) implies an addition of a link \( p_{22} = 0 + 0.5 \times 0.4 = 0.2 \) and the addition of \( 0.5 \times 4 = 2 \) on \( (F_0)_2 \) to get the equality:
\[ X([[0,0.5],[0.4,0]], [4,1]) = X([[0,0],[0.4,0.2]], [4,3]) \]

If we continue on suppressing the diagonal link \( p_{22} \), we get:
\[ X([[0,0],[0.4,0.2]], [4,3]) = X([[0,0],[0.4,0]], [4,3.75]) \]

Therefore, we get: \( X = [4 + 0.4 \times 3.75, 3.75] = (6, 3.75) \).

The above link suppression operation can be compared to the direct Gauss elimination method to solve \( A \cdot X = B \) (in
both cases, we get the exact limit in a finite number of operations). The possibility of applying such a links elimination method in the computation cost reduction of the eigenvector problem or to solve the linear equation \( A.X = B \) may be an interesting question. As the above illustration example shows, we can apply up to the point the solution \( X \) becomes explicit (no more links). However the cost of the link elimination is proportional to the number of incoming links and in the context of a very large matrix, such transformation may not be cost effective, because we may produce a very connected graph in the middle of the above transformation.

Also, it would be interesting to investigate further the idea of applying such a transformation for the purpose of nodes clustering problem.

Below, we show one application case of such a transformation.

### 3.3 Application of the graph transformation for the convergence condition

From \( P(c) \), we apply the diagonal suppression method. The result is \( Q \) such that:

\[
q_{ii} = 0
\]

and if \( i \neq j \):

\[
q_{ij} = \frac{-P(c)_{ij}}{1 - (P(c))_{ii}} = \frac{-a_{ij}}{a_{ii}}.
\]

The D-iteration for \( P(c) \) is convergent if and only if the D-iteration is convergent for \( Q \). As for the Gauss-Seidel iteration, the D-iteration converges when the spectral radius of \( Q \) is strictly less than 1.

**Remark 3.** The matrix \( Q \) may be obtained directly from \( A.X = B \), dividing each line \( i \) by \( a_{ii} \).

### 3.4 Another graph transformation

From \( A.X = B \), we can apply a more natural transformation for the fluid diffusion: because of the column based diffusion reduction condition, we set: \( x'_{i} = x_{i} \times a_{ii} \) and we divide by \( a_{ii} \) the \( i \)-th column vector of \( A \) to get \( A' \). Then we get \( Q' = I_{d} - A' \) such that:

\[
q'_{ii} = 0
\]

and if \( i \neq j \):

\[
q'_{ij} = \frac{-a_{ij}}{a_{jj}}.
\]

The advantage of this approach is that this formulation is simpler to be taken into account for the sequence \( I \) optimization: for instance, for the greedy one step vision optimization (cf. Section [3]).

### 3.5 Example

To illustrate the different approaches and for a simple comparison, we introduce the following case:

\[
A = \begin{pmatrix}
5 & 3 & 2 & 0 \\
0 & 7 & -4 & 1 \\
-2 & 0 & 8 & 0 \\
0 & -2 & 1 & 3
\end{pmatrix}
\]

The results are shown on Figure [10]: we compared Jacobi, Power iteration (with \( c = 1/8 \)), Gauss-Seidel, D-iteration using \( Q \) with cyclical sequence \( I = 1, 2, 3, 4, 1, 2... \) (D-iter/Q: CYC) and D-iteration with greedy approach taking the node with the maximum fluid in absolute value (D-iter/Q: Greedy).

For the D-iteration, we assumed here that \( N \) diffusions are equivalent to one matrix-vector product iteration. We would get the same result considering a finer iteration cost count based on the number of link \( a_{ij} \) utilization.

![Figure 10: Convergence comparison.](image)

To illustrate further the impact of the choice of the sequence \( I \), we added in Figure [11] the result obtained when applying the D-iteration on \( Q' \) when taking the node that maximizes step by step the \( L_{1} \)-norm of \( F_{i+1} \), or equivalently the fluid reduction in one step (D-iter/Q': Greedy).

This example is only for illustration: in this particular case, the gain brought by the D-iteration is of the order of the gain brought by the Gauss-Seidel compared to the Jacobi iteration.

A much larger gain with D-iteration is expected with large sparse matrix and [10] gives an illustration of this in the context of PageRank on the web graph. And more importantly, we can efficiently and naturally distribute the proposed method.

### 4. OPEN PROBLEMS

#### 4.1 Optimization problem
problem or for a faster convergence when mixed with the iteration methods.

REMARK 4. It is interesting to notice that $X(P, F_0 - P, F_0) = F_0$. This is obvious from the algebraic power series formulation of $X$, but not that obvious from the point of view of the diffusion.

5. CONCLUSION

In this paper, we presented the D-iteration method, initially introduced in the PageRank eigenvector problem, to solve efficiently the linear equation $AX = B$.

We believe that we have here a promising new intuitive representation and approach that can be applied in a very large scope of linear problems.

Acknowledgments

The author is very grateful to François Baccelli for taking time with patience to follow-up this work from the beginning. The author wishes to thank also Bruno Aidan, Paul Labrégère and Gérard Burnside for their constant support. Great thanks to Fabien Mathieu and Stéphane Gaubert who put me on the track of the Gauss-Seidel iteration. Finally, a heartfelt thank to Suong Mai for her unconditional support.

6. REFERENCES

[1] S. Abiteboul, M. Preda, and G. Cobena. Adaptive on-line page importance computation. WWW2003, pages 280–290, 2003.

[2] A. Arasu, J. Novak, J. Tomlin, and J. Tomlin. Pagerank computation and the structure of the web: Experiments and algorithms, 2002.

[3] R. Bagnara. A unified proof for the convergence of jacobi and gauss-seidel methods. SIAM Review, 37, 1995.

[4] G. H. Golub and C. F. V. Loan. Matrix Computations. The Johns Hopkins University Press, 3rd edition, 1996.

[5] D. Hong. Optimized on-line computation of pagerank algorithm. submitted, 2012.

[6] C. Kohlschütter, P.-A. Chirita, R. Chirita, and W. Nejdl. Efficient parallel computation of pagerank. In Proc. of the 28th European Conference on Information Retrieval, pages 241–252, 2006.

[7] A. N. Langville and C. D. Meyer. Deeper inside pagerank. Internet Mathematics, 1(3), 2004.

[8] L. Page, S. Brin, R. Motwani, and T. Winograd. The pagerank citation ranking: Bringing order to the web. Technical Report Stanford University, 1998.

[9] Y. Saad. Iterative Methods for Sparse Linear Systems. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2nd edition, 2003.