Numer. Math. 42, 161-172 (1983)



Solution of Underdetermined Nonlinear Equations by Stationary Iteration Methods

Klaus-Hermann Meyn

BASF AG, Abt. DFI/ND, D-6700 Ludwigshafen (Fed. Rep.)

Summary. Nonlinear stationary fixed point iterations in R^n are considered. The Perron-Ostrowski theorem [23] guarantees convergence if the iteration function G possesses an isolated fixed point u. In this paper a sufficient condition for convergence is given if G possesses a manifold of fixed points.

As an application, convergence of a nonlinear extension of the method of Kaczmarz is proved. This method is applicable to underdetermined equations; it is appropriate for the numerical treatment of large and possibly ill-conditioned problems with a sparse, nonsquare Jacobian matrix. A practical example of this type (nonlinear image reconstruction in ultrasound tomography) is included.

Subject Classifications: AMS(MOS) 65H10; CR 5.15.

1. Introduction

Let $D \subset \mathbb{R}^n$ be an open set; let $G: D \to \mathbb{R}^n$ be a continuous mapping. The subject of this paper are nonlinear stationary processes of the type

(1.1)
$$x^{k+1} = G(x^k);$$

G is assumed to possess a manifold of fixed points where possibly the spectral radius of G' satisfies $\rho(G'(u))=1$. This case is not covered by the Perron-Ostrowski theorem [23].

Linear processes of this kind have been investigated by a number of authors, e.g. Oldenburger [21], Ansorge [2], Keller [16], Tanabe [29]. For a real or complex $n \times n$ -matrix Q let

(1.2)
$$x^{k+1} = Qx^k + b,$$

where b is such that u=Qu+b is consistent. The scheme (1.2) converges if and only if any of the following four conditions is satisfied:

$$\lim_{i\to\infty} Q^i \text{ exists};$$

(1.4) for any eigenvalue λ of Q either $|\lambda| < 1$ or $\lambda = 1$; every elementary divisor for an eigenvalue 1 is linear (Ansorge [2]);

(1.5) $R^n = N_1 \bigoplus N_2$; N_1 and N_2 are invariant subspaces of Q; Q is the identity on N_1 and convergent on N_2 (Keller [16]);

(1.6) $\rho(Q|_{Im(I-Q)}) < 1$ (Tanabe [29]).

In (1.6), I is the $n \times n$ identity matrix, Im(I-Q) denotes the range of I-Q and $Q|_{I-Q}$ is the restriction of the mapping Q to Im(I-Q).

In this framework, Tanabe [28] has shown that the method of Kaczmarz [14] converges for (practically) every linear system of equations, regardless if there exists a variety of solutions or no solution at all. Other convergence results have been obtained by Herman and his coworkers [11], McCormick [18], and Elfving [6] for a block-iterative version. The popularity of the method in problems like image reconstruction (Gordon et al. [9]) and image restoration (Huang [12]) is mainly due to its computational simplicity and to the fact that sparsity of the corresponding matrices can easily be exploited.

For nonlinear systems of equations, a combination of the Kaczmarz method as primary iteration together with the one-dimensional Newton method as secondary iteration has been proposed by Tompkins [30]. It is shown that this and some related methods converge locally if the corresponding system of equations possesses a manifold of solutions.

In the final section, a brief introduction to the image reconstruction problem in ultrasound tomography is given. This amounts to the numerical solution of an inverse problem for a wave equation. The continuous problem is ill-posed and frequently underdetermined. A discretization will reflect these properties. Using an algorithm derived by Schomberg [26], it is demonstrated that collocation and subsequent application of the Kaczmarz-Newton method, together with a simple regularization provide an efficient technique for its numerical inversion.

The following notation will be used: For a matrix A, A^* is the adjoint and Ker A is the nullspace. $N(x, \varepsilon)$ is an ε -neighbourhood of a point $x \in \mathbb{R}^n$ with respect to the Euclidean norm $\|\cdot\|$.

2. Convergence of Fixed Point Iteration in the Presence of a Manifold of Fixed Points

For the mapping G defined in Sect. 1, suppose that

$$E = \{u \mid u = G(u)\} \subset D$$

is a manifold of fixed points. For every $x \in D$ let there be a $u(x) \in E$ such that

$$||x-u(x)|| = \min_{u\in E} ||x-u||;$$

the mapping $x \rightarrow u(x)$ is assumed to be continuous.

(1.3)

Lemma 2.1. Suppose that for an $u^0 \in E$ there is an $N(u^0, \varepsilon)$ and an $\alpha < 1$ such that

$$||G(x) - u(x)|| \le \alpha ||x - u(x)||$$

for all $x \in N(u^0, \varepsilon)$. Then there is an $N(u^0, \delta) \subset N(u^0, \varepsilon)$ such that for every starting vector $x^0 \in N(u^0, \delta)$ the sequence $\{x^k\}$ generated by (1.1) satisfies

$$\lim_{k\to\infty} x^k = u \in E \cap N(u^0, \varepsilon).$$

Proof. δ can be chosen so that for any $x^0 \in N(u^0, \delta)$

$$\frac{1+\alpha}{1-\alpha} \|x^0 - u(x^0)\| + \|u(x^0) - u^0\| \leq \varepsilon.$$

The following two relations are easily proved by induction $(k \ge 1)$:

$$\begin{aligned} \|x^{k} - u(x^{k-1})\| &\leq \alpha^{k} \|x^{0} - u(x^{0})\|, \\ \|x^{k} - u^{0}\| &\leq \|x^{k} - u(x^{k-1})\| + \|x^{k-1} - u(x^{k-1})\| + \|x^{k-1} - u^{0}\| \\ &\leq (1+\alpha) \sum_{i=0}^{k-1} \alpha^{i} \|x^{0} - u(x^{0})\| + \|u(x^{0}) - u^{0}\|. \end{aligned}$$

Consequently, $\{x^k\} \subset N(u^0, \varepsilon)$, and every accumulation point of $\{x^k\}$ is a fixed point of G. Uniqueness of the accumulation point is a consequence of

$$\|x^{p} - x^{q}\| \leq \sum_{i=1}^{p-q} [\|x^{q+i} - u(x^{q+i-1})\| + \|x^{q+i-1} - u(x^{q+i-1})\|]$$
$$\leq \frac{2\alpha^{q}}{1-\alpha} \|x^{0} - u(x^{0})\|, p > q > 1,$$

which can be proved by the previous two inequalities. \Box

The following theorem generalizes some aspects of the Perron-Ostrowski theorem on the convergence of stationary iterative processes ([23, 22]).

Theorem 2.2. Suppose G is continuously differentiable in E. Let for an $u^0 \in E$

(2.1)
$$||G'(u^0)|_{\operatorname{Im}(I-G'(u^0))^*}|| = \beta < 1,$$

(2.2) for any $x \in D$ satisfying $u(x) = u^0 x - u^0 \in \text{Im}(I - G'(u^0))^*$.

Then there is an $N(u^0, \delta)$ such that for any starting vector $x^0 \in N(u^0, \delta) \{x^k\}$ satisfies

$$\lim_{k\to\infty} x^k = u \in E.$$

Proof. For all $x \in D$ with $u(x) = u^0$ evidently

$$\|G'(u^0)(x-u^0)\| \le \beta \|x-u^0\|$$

holds. Since G'(u(x)) is continuous, there exist $\varepsilon > 0$, $\beta^1 < 1$ such that

(2.3)
$$||G'(u(x))(x-u(x))|| \le \beta^1 ||x-u(x)||$$

for all $x \in N(u^0, \varepsilon)$. For sufficiently small ε ,

(2.4)
$$||G(x) - G(u(x)) - G'(u(x))(x - u(x))|| \le \gamma ||x - u(x)||$$

with $\gamma < 1 - \beta^1$ for all $x \in N(u^0, \varepsilon)$. (2.3) and (2.4) yield $||G(x) - u(x)|| \leq (\gamma + \beta^1) ||x - u(x)||$, and Lemma 2.1 holds. \Box

If $I - G'(u^0)$ is nonsingular, then (2.2) is satisfied and (2.1) reduces to $||G'(u^0)|| < 1$, which is a stronger assumption than the one in the Perron-Ostrowski theorem. Also, if G is an affine function, then Theorem 2.2 is more restrictive than any of the conditions (1.3)-(1.6).

Condition (2.2) means in geometrical term that $x - u^0$ is orthogonal to the nullspace of $I - G'(u^0)$. Since $G: D \to \mathbb{R}^n$, the Jacobian matrix $I - G'(u^0)$ will generally be rank-deficient, and thus (2.2) is not at all obvious.

As an easy consequence of the preceding proof we note that the R_1 convergence factor (Ortega and Rheinboldt [22, p. 288]) can be estimated by

$$R_{1}\{x^{k} - u(x^{k})\} = \limsup_{k \to \infty} ||x^{k} - u(x^{k})||^{1/k}$$
$$\leq \rho(G'(u)|_{\mathrm{Im}(I - G'(u))^{*}}).$$

3. Convergence of a Nonlinear Extension of the Method of Kaczmarz

The algorithm described in this section is applicable to nonlinear equations

(3.1)
$$F(x) = \begin{pmatrix} f_1(x) \\ \vdots \\ f_m(x) \end{pmatrix} = 0,$$

where $F: D \rightarrow R^m$ is continuously differentiable in the open set $D \subset R^n$. There may exist a manifold of solutions of (3.1); *m* and *n* are arbitrary. Let

(3.2)
$$g_i(y) = y - f_i(y) \|\nabla f_i(y)\|^{-2} \nabla f_i(y), \quad i = 1, ..., m$$

 $(\nabla f_i \text{ denotes the gradient of } f_i \text{ and } \nabla f_i(y) \neq 0 \text{ is assumed})$. Starting from an initial vector x^0 , the nonlinear Kaczmarz method generates a sequence $\{x^k\}$ by the recursion $x^{k+1} = G(x^k)$, where

$$G(x) = g_m(\dots g_1(x) \dots)$$

This algorithm belongs to the class of generalized SOR-Newton-schemes considered by Ortega and Rheinboldt [22, p. 226]. Each computation of $g_i(y)$ amounts to a shift of y in the direction of $-Vf_i(y)$ towards the manifold $\{x | f_i(x)=0\}$. The steplength is determined in an obvious manner by one step of the one-dimensional Newton method. Alternatively, one step of the iteration can be interpreted as a sequence of orthogonal projections of the points $x^{k,i}$ $=g_i(x^{k,i-1}), x^{k,0}=x^k$ onto the hyperplanes $f_i(x^{k,i})+(\nabla f_i(x^{k,i}), x-x^{k,i})=0, i = 1, ..., m$. To the authors knowledge, this method is due to Tompkins [30] and was rediscovered by McCormick [18]. There exist similar methods for the solution of the convex feasibility problem, see Eremin [7], Raik [25], Censor and Lent [5] and the survey [3] of Censor. The proofs of convergence in these papers do not treat the case that (3.1) possesses a nonconvex set of solutions.

The Kaczmarz-Newton method is a row action method in the sense of [3], i.e. in every substep access is required to only one row of the Jacobian matrix and only one iterate has to be stored. This property makes the method attractive for the numerical treatment of very large and sparse problems.

In order to apply Theorem 2.2 we cite in the following Lemma two results of Tanabe on the linear Kaczmarz method ([28, Cor. 4, Th. 5.2]).

Lemma 3.1. Suppose A is a real or complex $m \times n$ -matrix and a_i is the *i*-th column vector of A^* . It is assumed that $||a_i|| \neq 0$ for i = 1, ..., m. The matrix Q is defined as follows:

$$Q = \prod_{i=m}^{1} (I - a_i a_i^* ||a_i||^{-2}).$$

Then $\operatorname{Ker}(I-Q) = \operatorname{Ker} A$ and $||Q|_{\operatorname{Im} A^*}|| < 1$.

Theorem 3.2. Suppose there is an $u^0 \in E$ such that G is well-defined in an ε -neighborhood $N(u^0, \varepsilon)$. For every $x \in D$ satisfying $u(x) = u^0$ we assume

(3.4)
$$x - u^0 \in \operatorname{Im} F'(u^0)^*.$$

Then there is a δ -neighbourhood such that the sequence $\{x^k\}$ converges for every starting vector $x^0 \in N(u^0, \delta)$ towards a $u \in N(u^0, \varepsilon) \cap E$.

Proof. The chain rule yields $G'(u^0) = \prod_{i=m}^{l} g'_i(u^0)$. A simple calculation shows that

$$g'_i(y) = I - \|\nabla f_i(y)\|^{-2} \nabla f_i(y) \nabla f_i(y)^*$$

for $f_i(y) = 0$. Lemma 3.1 with $A = F'(u^0)$ and $Q = G'(u^0)$ yields $\operatorname{Im} F'(u^0)^* = \operatorname{Im}(I - G'(u^0))^*$ and Theorem 2.2 holds because of

$$\|G'(u^0)|_{\operatorname{Im}(I-G'(u^0))^*}\| = \|G'(u^0)|_{\operatorname{Im}F'(u^0)^*}\| < 1.$$

Assumption (3.4) is for instance satisfied if there exist – possibly after a suitable permutation of indices – functions $\{f_1, ..., f_m\} \subset \{f_1, ..., f_m\}$ with the property

(3.5)
$$\operatorname{rank} F'(u) = m' = \operatorname{rank} \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(u), \dots, \frac{\partial f_1}{\partial x_n}(u) \\ \dots \\ \frac{\partial f_{m'}}{\partial x_1}(u), \dots, \frac{\partial f_{m'}}{\partial x_n}(u) \end{pmatrix}$$

for all $u \in N(u^0, \varepsilon)$. According to some well-known results of analysis (e.g. Ostrowski [24, §16, 79]), $\{f_{m'+1}, \ldots, f_m\}$ are dependent on $\{f_1, \ldots, f_{m'}\}$ in the following way:

(3.6)
$$f_i(u) = \psi_i(f_1(u), \dots, f_{m'}(u)), \quad m' + 1 \leq i \leq m,$$

where $\psi_i: \mathbb{R}^{m'} \to \mathbb{R}^1$ and $u \in N(u^0, \varepsilon)$. For all $u \in D$ satisfying $f_1(u) = \ldots = f_{m'}(u) = 0$, (3.6) shows that

(3.7)
$$f_i(u) = f_i(u^0) = 0, m' + 1 \le i \le n$$

Therefore, if x satisfies $||x-u^0||^2 = \min \{||x-u||^2 | F(u)=0\}$, then also

(3.8)
$$||x-u^0||^2 = \min\{||x-u||^2 | f_1(u) = ... = f_{m'}(u) = 0\}.$$

Standard Lagrange multiplier theory for (3.8) finally yields (3.4).

4. Convergence of Other Methods

Theorem 4.1. Under the same assumptions on F as in Theorem 3.2 the following methods converge:

(a) the Kaczmarz-Newton method with relaxation, i.e. g_i is defined by

(4.1)
$$g_i(y) = y - \omega f_i(y) \|\nabla f_i(y)\|^{-2} \nabla f_i(y), 0 < \omega < 2;$$

(b) the corresponding simultaneous iteration scheme of Hart and Motzkin [10]

(4.2)
$$x^{k+1} = x^k - \sum_{i=1}^m \omega_i f_i(x^k) \| \nabla f_i(x^k) \|^{-2} \nabla f_i(x^k)$$

for $\omega_i > 0, \sum \omega_i < 2;$

(c) the method of Altman [1]

(4.3)
$$x^{k+1} = x^k - \omega F'(x^k) \|F'(x^k)\|^{-2} F(x^k), 0 < \omega < 2.$$

Proof. (a) Following the reasoning of Tanabe [28], it is possible to prove an extension of Lemma 3.1 where Q is replaced by $\prod (I - \omega a_i a_i^* ||a_i||^{-2})$, $0 < \omega < 2$. The rest is a mere repetition of the proof of Theorem 3.2

(b) A block-iterative version of (4.2) for systems of linear equations was considered by Elfving [6]. If

$$G(y) = y - \sum_{i=1}^{m} \omega_i f_i(y) \| \nabla f_i(y) \|^{-2} \nabla f_i(y),$$

then

$$G'(y) = I - \sum_{i=1}^{m} \omega_i \nabla f_i(y) \nabla f_i(y)^* \| \nabla f_i(y) \|^{-2} \quad \text{for } f_i(y) = 0, \ i = 1, \dots, m.$$

Since G'(y) is Hermitian,

$$\|G'(u)|_{\operatorname{Im}(I-G'(u))^*}\| = \rho(G'(u)|_{\operatorname{Im}(I-G'(u))} < 1$$

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because of [6, Th. 9]. It should be noted that according to Elfving the conditions on ω_i can be relaxed.

(c) This can be proved in a similar way as (b) using results of Friedrich [8]. The method of Altman has been thoroughly investigated by McCormick [17].

5. Numerical Solution of a Nonlinear Image Reconstruction Problem Arising in Ultrasound Tomography

Ultrasound tomography is a technique for obtaining a tomographic image of the internal structure of an object via ultrasound time-of-flight measurements in a similar way as in computed tomography with X-rays (Kak [15]). It is hoped that ultrasound tomography will become relevant for the early detection of breast cancer.

At the very beginning, the well-proven reconstruction techniques of X-ray CT were applied to ultrasound CT. Soon it was recognized that the results obtained in this way were poor since ultrasound – in contrast to X-rays – does not propagate along straight "rays". A more adequate physical model for ultrasound is geometrical acoustics, i.e. the rays – according to Fermat's principle – are curved in a way that depends on the object to be investigated. The function n which represents the unknown object is called the acoustical refractive index (following the notation of the references, n does not denote a dimension). For a parallel scanning geometry and a refractive index depending on two space variables, the problem can be posed as follows: Let

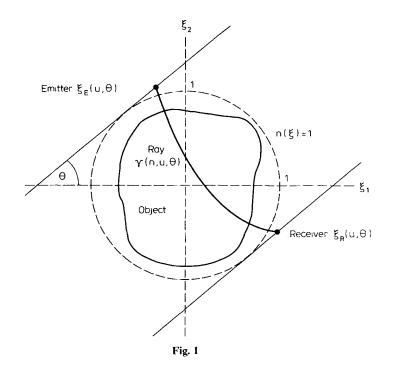
$$\xi_E(u,\theta) = \begin{vmatrix} u\cos\theta - \sin\theta \\ u\sin\theta + \cos\theta \end{vmatrix}, \quad \xi_R(u,\theta) = \begin{vmatrix} u\cos\theta + \sin\theta \\ u\sin\theta - \cos\theta \end{vmatrix}$$

for $-\infty < u < \infty$, $0 \le \theta < \pi$. For fixed $\theta, \xi_E(u, \theta)$ (the emitter position) and $\xi_R(u, \theta)$ (the receiver position) are a pair of parallel lines tangent to the unit circle (Fig. 1).

Let $n: \mathbb{R}^2 \to \mathbb{R}$ be a positive function with $n(\xi) = 1$ for $\|\xi\| \ge 1$; and let n possess all the smoothness properties required in the sequel. Let $\gamma(n, u, \theta)$ be the path of an ultrasound ray passing from the emitter $\xi_E(u, \theta)$ to the receiver $\xi_R(u, \theta)$. For nonconstant $n, \gamma(n, u, \theta)$ is not a straight line, but is determined by the variational principle

(5.1)
$$\int_{\gamma} n ds = \min;$$

where γ is a curve connecting $\xi_E(u, \theta)$ and $\xi_R(u, \theta)$, and ds denotes the line element of arc length. If several such rays exist (possibly corresponding to local minima of (5.1)), let $\gamma(n, u, \theta)$ be one for which (5.1) attains an absolute minimum. The line integral (5.1) is – up to a normalization factor – the time-offlight of an ultrasound pulse travelling along $\gamma(n, u, \theta)$. Since these time-offlights can be measured, the reconstruction problem in its continuous form is to recover *n* from the nonlinear integral equation



(5.2)
$$\int_{\gamma(n,u,\theta)} n ds = h(u,\theta), -\infty < u < \infty, 0 \le \theta < \pi.$$

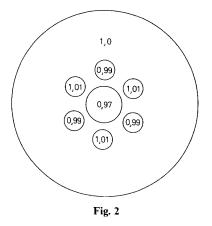
This so-called inverse kinematic problem for the wave equation $n^2 u_{rt} = \Delta u$ is for a different scanning geometry the classical inverse problem of seismology. It is well-known that even the continuous problem is not necessarily uniquely solvable. (Gilbert and Johnson [13], McKinnon and Bates [19]; a condition for uniqueness is given by Muhometov [20].) The well-established methods of solution like the Backus-Gilbert-technique ([13]) are too time-consuming for medical applications. Schomberg introduced in [26] a nonlinear extension of the Algebraic Reconstruction technique, basically a special kind of collocation with subsequent application of the Kaczmarz-Newton method which we are going to describe now.

The time-of flight data $h(u, \theta)$ are in practice measured at a discrete set of points (u_l, θ_p) , $1 \le 1 \le L$, $1 \le p \le P$. The refractive index *n* is approximated by a finite set of linear independent functions $\{\phi_i/1 \le i \le m\}$:

$$n \approx \tilde{n} = \sum_{i=1}^{m} x_i \phi_i.$$

For a fixed *m*-tupel $x = (x_1, ..., x_m)$, the ray passing from the emitter $\xi_E(u_1, \theta_p)$ to the receiver $\xi_R(u_1, \theta_p)$ (with respect to \tilde{n}) can be computed by the numerical solution of the variational problem

$$\int_{\gamma(\tilde{n}, u_l, \theta_p)} \tilde{n} ds = \min !$$



The numerical approximation of $\gamma(\tilde{n}, u_1, \theta_p)$ will be denoted by $\tilde{\gamma}(\tilde{n}, u_1, \theta_p)$. Using a suitable quadrature scheme, the line integrals can be evaluated:

$$\left(\int_{\tilde{\gamma}(\tilde{n},u_{l},\theta_{p})}\phi_{1}\,ds,\ldots,\int_{\tilde{\gamma}(\tilde{n},u_{l},\theta_{p})}\phi_{m}ds\right)\approx\left(a_{1}^{lp}(x),\ldots,a_{m}^{lp}(x)\right).$$

Thus, we arrive via collocation at the following discrete ill-conditioned counterpart of (5.2):

$$\int_{\mathcal{Y}(\tilde{n}, u_l, \theta_p)} \tilde{n} ds \approx (a^{lp}(x), x) = h(u_l, \theta_p), \ 1 \leq l \leq L, \ 1 \leq p \leq P.$$

This nonlinear system of equations can be solved by the Kaczmarz-Newton method of §3; details of the algorithm like the computation of the derivatives and regularization are given in [27].

The time-of-flight data of the following numerical example were experimentally measured for 75 uniformly spaced angles θ_p , $0 \leq \theta_p < \pi$, and for 64 uniformly spaced positions u_i , $-1 \leq u_i \leq 1$. The object consisted of 7 thin-walled rubber tubes filled with saline and hanging in a water tank. The refractive index of this phantom varied as indicated in Fig. 2. The problem was discretized by bilinear finite elements on an even 64×64 -grid. Starting from the initial guess n=1, three cycles of the Kaczmarz-Newton method were performed. In Fig. 3, a grey-scale image of the reconstruction is shown.

The problem as seetched above applies to a refractive index depending on two space variables. For medical applications, n depends on three space variables, and the rays are curved in \mathbb{R}^3 . In this situation, additional measurements in vertical direction have to be made. Let the position of the emitter/receiver pair be described by

$$\xi_E(u,\theta,z) = \begin{vmatrix} u\cos\theta - \sin\theta \\ u\sin\theta + \cos\theta \\ z \end{vmatrix}, \ \xi_R(u,\theta,z) = \begin{vmatrix} u\cos\theta + \sin\theta \\ u\sin\theta - \cos\theta \\ z \end{vmatrix},$$

where z is the vertical position. If $\gamma(n, u, \theta, z)$ is the path of the ultrasound ray passing from the emitter $\xi_E(u, \theta, z)$ to the receiver $\xi_R(u, \theta, z)$ and if $h(u, \theta, z)$ is

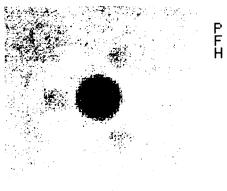


Fig. 3

the corresponding time-of-flight, then n is to be recovered from the following equation even if one is only interested in one slice of n:

$$\int_{\gamma(n,u,\theta,z)} n\,ds = h(u,\theta,z).$$

In the following numerical example, a three-dimensional refractive index varying between 0.95 and 1.05 was generated on a computer. This is about the range of soft human tissue. Measurements for 45 evently spaced angles θ_p , 64 evenly spaced emitter/receiver pairs with lateral position u_l , and 10 layers z_q were simulated. After introducing 0.5% random artificial noise to the data, the problem was solved in a similar way as in the 2-dimensional case (trilinear elements on an even grid, approximately 22,000 unknowns and 28,000 equations). Figure 4 shows the middle layer of the original phantom and Fig. 5 the reconstruction of the same layer after three cycles of the Kaczmarz-Newton method.

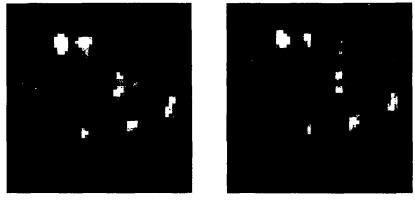


Fig. 4



Acknowledgement. This paper was written at the Philips Research Laboratory in Hamburg. I thank my former colleagues H. Schomberg, H.J. Schneider, D. Havixbeck and B. Fink for helpful discussions and help with the programming. Special thanks are due to B. Werner for pointing out to me some shortcomings in an early version of the manuscript.

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Received October 1, 1980/November 26, 1982/April 27, 1983