Scale-Space Properties of Regularization Methods

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Abstract. In this paper we show that regularization methods form a scale-space where the regularization parameter serves as scale. In analogy to nonlinear diffusion filtering we establish continuity with respect to scale, causality in terms of a maximum–minimum principle, simplification properties by means of Lyapunov functionals and convergence to a constant steady-state. We identify nonlinear regularization with a single implicit time step of a diffusion process. This implies that iterated regularization with small regularization parameters is a numerical realization of a diffusion filter. We present numerical experiments in two and three space dimensions illustrating the scale-space behaviour of regularization methods.

1 Introduction

There has often been a fruitful interaction between linear scale-space techniques and regularization methods. Torre and Poggio [29] emphasized that differentiation is ill-posed in the sense of Hadamard, and applying suitable regularization strategies approximates linear diffusion filtering or – equivalently – Gaussian convolution. Much of the linear scale-space literature is based on the regularization properties of convolutions with Gaussians. In particular, differential geometric image analysis is performed by replacing derivatives by Gaussian-smoothed derivatives; see e.g. [8, 15, 26] and the references therein. In a very nice work, Nielsen et al. [16] derived linear diffusion filtering axiomatically from Tikhonov regularization, where the stabilizer consists of a sum of squared derivatives up to infinite order.

Nonlinear diffusion filtering can be regarded both as a restoration method and a scale-space technique [11, 20, 30]. When considering the restoration properties, natural relations between *biased* diffusion and regularization theory exist via the Euler equation for the regularization functional. This Euler equation can be regarded as the steady-state of a suitable nonlinear diffusion process with a bias term [19, 25, 5]. A popular specific energy functional arises from unconstrained total variation denoising [1, 4, 3]. Constrained total variation also leads to a nonlinear diffusion process with a bias term using a time-dependent Lagrange multiplier [22].

When regarding nonlinear diffusion as a scale-space method we have to ensure that *architectural, invariance* and *simplification properties* exist [2]. A typical architectural property is continuity with respect to the scale parameter, a characteristic invariance property is the average grey level invariance, and simplification qualities can be stated in terms of a maximum–minimum principle, Lyapunov functionals and convergence to a constant steady-state [30].

Strong and Chan [28] proposed to regard the regularization parameter of total variation denoising as a scale parameter. However, a corresponding scale-space interpretation of regularization methods, which is in analogy to results for nonlinear diffusion scale-spaces, has been missing so far. This topic will be discussed in the present paper. We show that there exists a scale-space theory for regularization methods which resembles very much the one for nonlinear diffusion filtering. Following [13, 23, 28] we interpret the regularization parameter as a diffusion time by considering regularization as time-discrete diffusion filtering with a single implicit time step. Consequently, iteration of regularization with small regularization parameters can be regarded as an approximation to diffusion filtering.

Our paper is organized as follows: In Section 2 we survey scale-space properties of diffusion filtering. In Sections 3 and 4 an analogous theory for noniterated and iterated regularization techniques is established. Due to the lack of space we can survey only the main results. Proofs and full details can be found in technical reports [24, 21]. In Section 5 we present some experiments with 2D MR images and 3D ultrasound data, and compare the restoration properties of noniterated and iterated regularization.

2 Diffusion Filtering

In this section we review essential scale-space properties of nonlinear diffusion filtering. The presented results can also be extended to a broader class of methods including regularized filters with nonmonotone flux functions and anisotropic filters with a diffusion tensor. More details and proofs can be found in [30].

We consider a *diffusion process* of the form

$$\begin{cases} \partial_t u(x,t) = \nabla.\left(g(|\nabla u|^2)\nabla u\right)(x,t) & \text{on } \Omega \times [0,\infty[\\ \frac{\partial u}{\partial n}(x,t) = 0 & \text{on } \Gamma \times [0,\infty[\\ u(x,0) = f(x) & \text{on } \Omega\ . \end{cases} \tag{1}$$

The image domain $\Omega \subseteq \mathbb{R}^d$ is assumed to be bounded with piecewise Lipschitzian boundary Γ with unit normal vector n, and $f \in L^\infty(\Omega)$ is a degraded original image with $a := \operatorname{ess\,inf}_\Omega f$ and $b := \operatorname{ess\,sup}_\Omega f$.

The diffusivity g satisfies the following properties:

1. $g \in C^\infty([0,\infty))$
2. The flux $g(s^2)s$ is monotonically increasing in s.
3. $g(s) > 0$ for all $s \geq 0$.

Under these assumptions there exists a unique solution $u(x,t)$ of (1), such that $\|u(.,t)\|_{L^2(\Omega)}$ is continuous for $t \geq 0$. This continuity property is necessary for relating structures over scales and for retrieving the original image for $t \to 0$. It is one of the fundamental architectural ingredients of scale-space theory.

Moreover, the average grey level is conserved:

$$\frac{1}{|\Omega|} \int_\Omega u(x,t)dx = Mf \quad \text{for all } t > 0\,,$$

with

$$Mf := \frac{1}{|\Omega|} \int_\Omega f(x)\,dx\ .$$

A constant average grey level is essential for scale-space segmentation algorithms such as the hyperstack [17]. It is also a desirable quality in medical imaging where grey values measure physical quantities of the depicted object, for instance proton densities in MR images.

The unique solution of (1) fulfills the extremum principle

$$a \leq u(x,t) \leq b \text{ on } \Omega \times (0,T]. \tag{2}$$

The extremum principle is an equivalent formulation of Koenderink's causality requirement [12]. Together with the continuity it ensures that level sets can be traced back in scale.

Another important simplification property can be expressed in terms of Lyapunov functionals. For all $r \in C^2[a,b]$ with $r'' \geq 0$ on $[a,b]$, the function

$$V(t) := \phi(u(t)) := \int_\Omega r(u(x,t))\,dx \tag{3}$$

is a Lyapunov functional since it satisfies

1. $\phi(u(t)) \geq \phi(Mf)$ for all $t \geq 0$
2. (a) $V \in C[0,\infty) \cap C^1(0,\infty)$
   (b) $V'(t) \leq 0$ for all $t > 0$.

Lyapunov functionals show that diffusion filters create simplifying transformations: the special choices $r(s) := |s|^p$, $r(s) := (s - Mf)^{2n}$ and $r(s) = s\ln(s)$, respectively, imply that all L^p norms with $p \geq 2$ are decreasing, all even central moments are decreasing, and the entropy $S[u(t)] := -\int_\Omega u(x,t)\ln u(x,t)\,dx$, a measure of uncertainty and missing information, is increasing with respect to

t. Lyapunov functionals have been used for scale-selection and texture analysis [27], for the synchronisation of different diffusion scale-spaces [17], and for the automatic determination of stopping times [31]. Moreover, they allow to prove that the filtered image converges to a constant image as t tends to ∞: $\lim_{t\to\infty} \|u(t) - Mf\|_{L^p(\Omega)} = 0$ for $p \in [1, \infty)$. For $d = 1$ we have even uniform convergence.

3 Regularization

An interesting relation between nonlinear diffusion filtering and regularization methods becomes evident when considering an implicit time discretization [13, 23, 28]. The first step of an implicit scheme with step-size h in t–direction reads as follows.

$$\begin{cases} \frac{u(x,h)-u(x,0)}{h} = \nabla.\left(g(|\nabla u|^2)\nabla u\right)(x,h) \\ \frac{\partial u}{\partial n}(x,h) = 0 \\ u(x,0) = f(x)\ . \end{cases} \tag{4}$$

In the following we assume the existence of a differentiable function $\hat{g}$ on $[0,\infty)$ which satisfies $\hat{g}' = g$. Then the minimizer of the functional

$$T(u) := \|u - f\|^2_{L^2(\Omega)} + h \int_\Omega \hat{g}(|\nabla u|^2)\,dx\,, \tag{5}$$

satisfies (4). If the functional T is convex, then a minimizer of T is uniquely characterized by the solution of equation (4).

$T(u)$ is a typical regularization functional consisting of the approximation functional $\|u - f\|^2_{L^2(\Omega)}$ and the stabilizing functional $\int_\Omega \hat{g}(|\nabla u|^2)\,dx$. The weight h is called *regularization parameter*. An extensive discussion of regularization methods can be found in [7].

Now we present a scale-space theory for a broad class of regularization methods. For proofs and full details we refer to [24].

Let $\hat{g}$ satisfy:

1. $\hat{g}(.)$ is continuous for any compact $K \subseteq [0,\infty)$.
2. $\hat{g}(0) = \min\{\hat{g}(x) : x \in [0,\infty)\} \geq 0$.
3. $\hat{g}(|.|^2)$ is convex from $\mathbb{R}^d$ to $\mathbb{R}$.
4. There exists a constant $c > 0$ such that $\hat{g}(s) \geq cs$.
5. $\hat{g}$ is monotone in $[0,\infty)$.

These assumptions guarantee existence and uniqueness of a minimizer u_h for the regularization functional (5) in the Sobolev space $H^1(\Omega)$. They are satisfied for the following regularization techniques:

1. Tikhonov regularization:

$$\hat{g}(|s|^2) = |s|^2\ .$$

2. The modified total variation regularization of Ito and Kunisch [14]:

$$\hat{g}(|s|^2) = \sqrt{|s|^2} + \alpha|s|^2, \text{ with } \alpha > 0 \ .$$

3. The modified total variation regularization of Nashed and Scherzer [18]:

$$\hat{g}(|s|^2) = \sqrt{|s|^2 + \beta^2} + \alpha|s|^2 \ .$$

4. The regularization of Geman and Yang [9] and Chambolle and Lions [4]:

$$\hat{g}(|s|^2) = \begin{cases} \frac{1}{2\varepsilon}|s|^2 & |s| \leq \varepsilon \\ |s| - \frac{\varepsilon}{2} & \varepsilon \leq |s| \leq \frac{1}{\varepsilon} \\ \frac{\varepsilon}{2}|s|^2 + \frac{1}{2}\left(\frac{1}{\varepsilon} - \varepsilon\right) & |s| > \frac{1}{\varepsilon} \ . \end{cases}$$

5. Schnörr's [25] convex nonquadratic regularization:

$$\hat{g}(|s|^2) = \begin{cases} \lambda_h^2|s|^2 & |s| \leq c_\rho \\ \lambda_l^2|s|^2 + (\lambda_h^2 - \lambda_l^2)c_\rho(2|s| - c_\rho) & |s| > c_\rho \ . \end{cases}$$

The assumption 4. on $\hat{g}$ is violated for

1. Green's functional [10]:

$$\hat{g}(|s|^2) = \ln(\cosh(|s|)^2) \ .$$

2. Total variation regularization [22]:

$$\hat{g}(|s|^2) = \sqrt{|s|^2} \ .$$

3. The regularization proposed by Acar and Vogel [1]:

$$\hat{g}(|s|^2) = \sqrt{|s|^2 + \beta^2} \ .$$

Moreover, the functional $\|u_h\|_{L^2(\Omega)}$ can be shown to be continuous in $h \geq 0$. This continuity property allows to relate structures over scales of regularization parameters.

In analogy to diffusion filtering, the average grey level invariance

$$\int_\Omega u_h \, dx \ = \int_\Omega f \, dx \quad \text{for all } h \geq 0$$

and the extremum principle

$$a \leq u_h \leq b \quad \text{for all } h \geq 0$$

can be established.

Moreover, Lyapunov functionals for regularization methods can be constructed in a similar way. For all $r \in C^2[a,b]$ with $r'' \geq 0$, the function

$$V(h) := \phi(u_h) := \int_\Omega r(u_h(x)) \, dx \tag{6}$$

is a Lyapunov functional:

1. $\phi(u_h) \geq \phi(Mf)$ for all $h \geq 0$.
2. (a) $V \in C[0,\infty)$,
   (b) $DV(h) := \int_\Omega r'(u_h)(u_h - u_0) \leq 0$, for all $h \geq 0$.
   (c) $V(h) - V(0) \leq 0$ for all $h \geq 0$.

Here, a difference between Lyapunov functionals for diffusion processes and regularization methods becomes evident. For Lyapunov functionals in diffusion processes we have $V'(t) \leq 0$, and in regularization processes we have $DV(h) \leq 0$. $DV(h)$ is obtained from $V'(t)$ by making a time discrete ansatz at time 0. We note that this is exactly the way we compared diffusion filtering and regularization techniques. It is therefore natural that the role of the time derivative in diffusion filtering is replaced by the time discrete approximation around 0.

Again, these Lyapunov functionals allow to prove convergence of the filtered images to a constant image as $h \to \infty$:

d=1: u_h converges uniformly to Mf for $h \to \infty$
d=2: $\lim\limits_{h\to\infty} \|u_h - Mf\|_{L^p(\Omega)} = 0$ for any $1 \leq p < \infty$
d=3: $\lim\limits_{h\to\infty} \|u_h - Mf\|_{L^p(\Omega)} = 0$ for any $1 \leq p \leq 6$

We observe that for $d = 3$ the convergence result is slightly weaker than in the diffusion case.

4 Iterated Regularization

Regularization can be applied iteratively where the regularized solution of the previous step serves as initial image for the next iteration. For small regularization parameters, iterated regularization becomes therefore a good approximation to a nonlinear diffusion filter.

Let us consider an iterative regularization process with positive regularization parameters h_k, $k = 1, ..., \infty$, such that the corresponding "diffusion time" $t_n := \sum_{k=1}^{n} h_k$ tends to ∞ for $n \to \infty$. The $n - th$ iteration reads as follows:

$$\begin{cases} \dfrac{u(x,t) - u(x,t_{n-1})}{t - t_{n-1}} = \nabla.\left(g(|\nabla u|^2)\nabla u\right)(x,t) \qquad t \in (t_{n-1}, t_n],\ x \in \Omega \\ \dfrac{\partial u(x,t)}{\partial n} = 0 \qquad x \in \Gamma \\ u(x,0) = f(x) \qquad x \in \Omega \end{cases} \tag{7}$$

where now $t - t_{n-1}$ serves as the regularization parameter in the interval $(t_{n-1}, t_n]$.

It is now possible to prove a similar scale-space theory as for noniterated regularization [21]. The main results are given below.

Under the same assumptions as for the noniterated case there exists a unique minimizer $u(\cdot,t)$. Moreover, the functional $\|u(\cdot,t)\|_{L^2(\Omega)}$ is continuous for $t \geq 0$. However, the spatial smoothness becomes better in each iteration step: after

n iterations the solution $u(.,t)$ is in the Sobolev space $H^{2n}(\Omega)$ for fixed $t \in (t_{n-1}, t_n]$. This suggests that, if one uses the regularized solution for calculating derivatives of order n, one should perform at least $n/2$ iterations.

As for noniterated regularization, the average grey level invariance and the extremum principle hold.

Even at the risk of boring the reader we introduce for the sake of completeness Lyapunov functionals for iterated regularization: for all $r \in C^2[a,b]$ with $r'' \geq 0$, the function

$$V(t) := \phi(u(.,t)) := \int_\Omega r(u(x,t))\,dx \tag{8}$$

is a Lyapunov functional:

1. $\phi(u(.,t)) \geq \phi(Mf)$ for all $t \geq 0$.
2. (a) $V \in C[0,\infty)$,
   (b) $DV(t) := \int_\Omega r'\,(u(x,t))\,(u(x,t) - u(x,t_{n-1})))\,dx \leq 0$, for all $t \in (t_{n-1}, t_n]$,
   (c) $V(t) - V(t_{n-1}) \leq 0$ for all $t \in (t_{n-1}, t_n]$.

In contrast to noniterated regularization, Lyapunov functionals for iterated regularization methods are based on the time discrete ansatz at $t = t_n$. Nevertheless, the convergence results from Section 3 carry over literally.

5 Experiments

The numerical experiments are performed using the software package DIFFPACK from the University of Oslo / Numerical Objects [6]. We have implemented the diffusion equation with diffusivity $\hat{g}(|\nabla u|^2) = \sqrt{|\nabla u|^2 + \beta^2} + \alpha|\nabla u|^2$ which is a modified total variation regularization. For this diffusion filtering our theoretical results are applicable. The term $\alpha|\nabla u|^2$ is only of theoretical interest; in numerical realizations, the discretized version of the gradient is bounded, and there is no visible difference between using very small values of α (in which the theoretical results are applicable) and $\alpha = 0$ (where our theoretical results do not hold).

Our experiments were carried out for different sequences of time-steps and various smoothing parameters β. The influence of the parameter settings is as follows.

The impact of β on the numerical reconstruction is hardly viewable in the range from $\beta = 10^{-2}$ to 10^{-4}. Even the convergence rate is, although slower for smaller β, hardly affected.

For small values of regularization parameters h (up to approximately 5.0), there is no visible difference between iterated and noniterated regularization. The effect can only be seen for larger values of h. This is illustrated in Figure 2. It shows the result of noniterated and iterated regularization applied to the 2D

MR image from Figure 1. The results are depicted at times $t = 10$, 30, and 100, respectively. For noniterated regularization this is achieved in one step, and for iterated regularization the regularization parameter $h = 1$ was chosen and 10, 30, or 100 iterations were performed. We observe that differences between the two methods are very small. They only become evident when subtracting one image data from the other and rescaling the difference into the interval $[0, 255]$. This also indicates that the semigroup property of regularization methods is well approximated in practice. It should be noted that the semigroup property is an ideal continuous concept which can only be approximated in time-discrete algorithms for partial differential equations.

original data

Fig. 1. The noisy MR-image of a head used as initial data.

As can be seen from the previous sections, the scale-space framework for regularization methods carries over to higher space dimensions. In the next figure we present results from a three-dimensional ultrasound data set of the upper abdomen with $80 \times 80 \times 80$ voxels. While the calculations were perfomed in three dimensions, we show a scale-space evolution of a single slice of the data set. The elimination of the speckle noise demonstrates that iterated regularization can handle very noisy real-world data without destroying important image features.

6 Conclusions

Traditionally, scale-space techniques have been linked to parabolic or hyperbolic partial differential equations [2]. The novelty of our paper consists of establishing a parameter dependent elliptic boundary value problem (noniterated regularization) and a sequence of elliptic problems (iterated regularization) as scale-space techniques. They satisfy the same scale-space properties as nonlinear diffusion filtering. The key ingredient for understanding this relation is the interpretation of regularization methods as time-implicit approximations to diffusion processes. In this sense, the scale-space theory of regularization methods is also a novel semi-discrete theory to diffusion filtering. This time discrete framework completes the theory of diffusion scale-spaces where up to now only results for the continuous, the space-discrete and the fully discrete setting have been formulated [30].

The synthesis of regularization techniques and diffusion methods may lead to a deeper understanding of both fields. In particular, it is likely that many more results can be transferred from one of these areas to the other.

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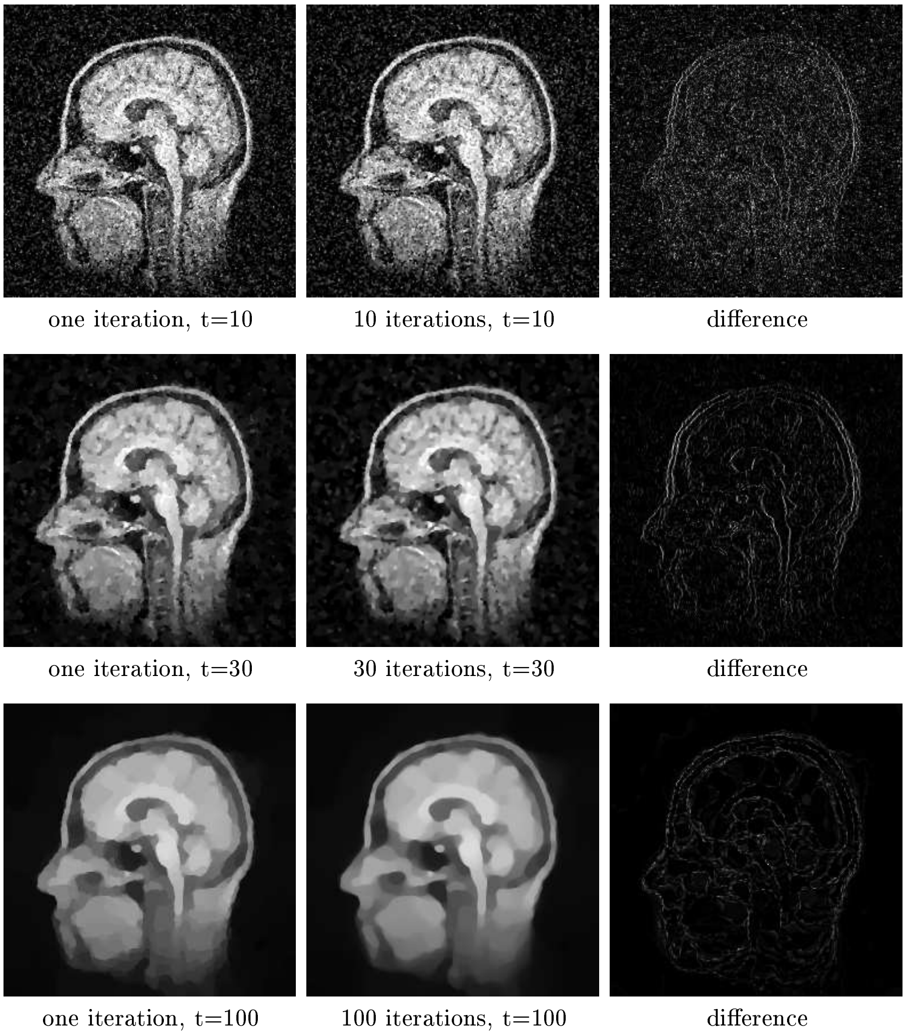
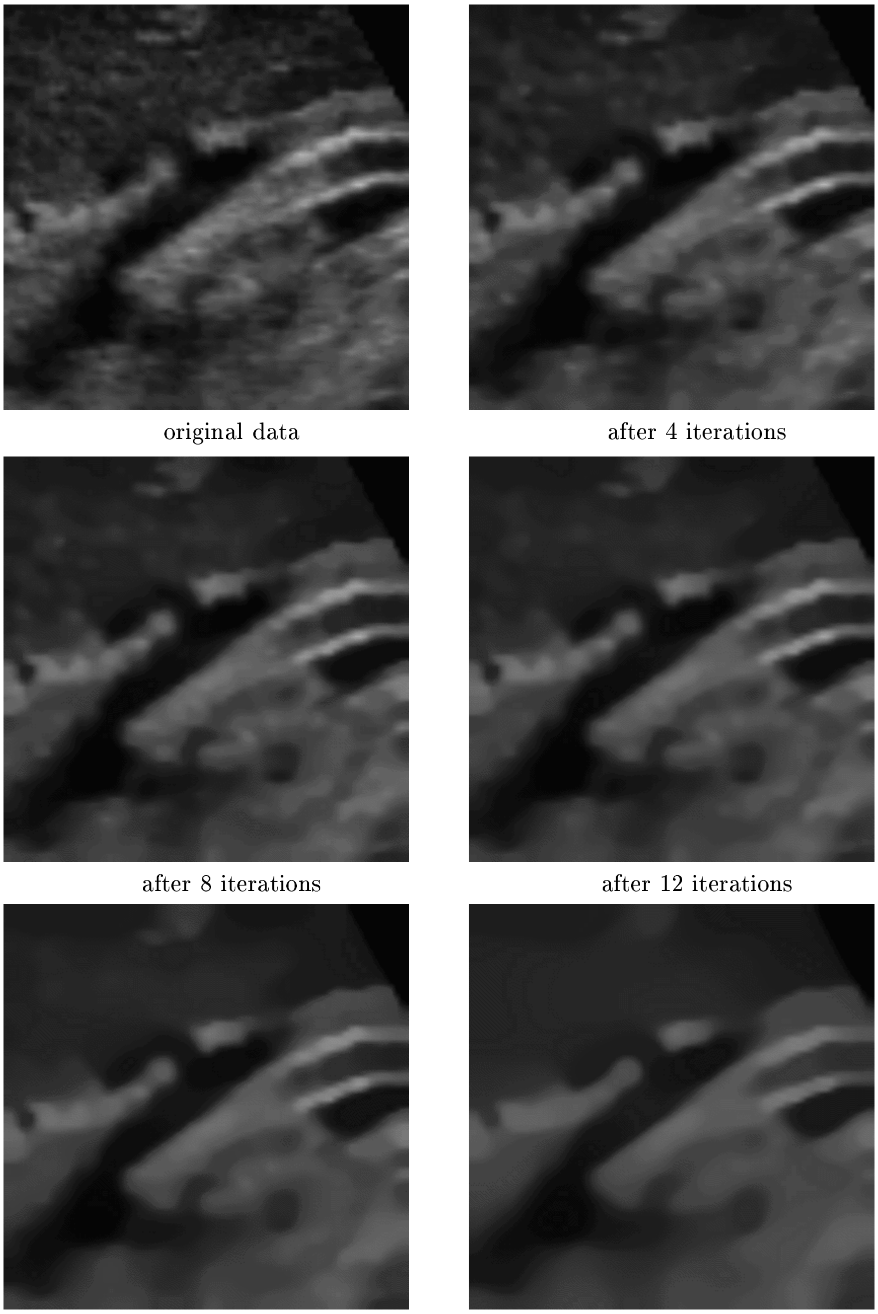


Fig. 2. Results for the MR-image of a head with noniterated and iterated regularization ($\beta = 0.001$). The left column shows the results for noniterated, the middle column for iterated regularization. The images in the right column are the differences between the results for the iterated and noniterated method; the contrast of the difference images is normalized to $[0, 255]$.



original data | after 4 iterations

after 8 iterations | after 12 iterations

after 20 iterations | after 40 iterations

Fig. 3. Results for the three-dimensional ultrasound data with $\beta = 0.001$ and regularization parameter $h = 0.5$.