Multiscale Methods for Polyhedral Regularizations

Michael Möller* Martin Burger*

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Abstract

In this paper we present the extension and generalization of the adaptive inverse scale space (aISS) method proposed for ℓ^1 regularization in [BMBO11] to arbitrary polyhedral functions. We will see that the representation of a convex polyhedral function as a finitely generated function yields a fast and general aISS algorithm. We analyze its convergence and interpret the well known (forward) scale space flow as the inverse scale space flow on the convex conjugate functional, thus including this class of flows in our analysis. A surprising result is the equivalence of the scale space or gradient flow with a standard variational problem. Finally, we give some examples of the applications for the adaptive inverse scale space algorithm for polyhedral functions.

Key words: Inverse Scale Space, Scale Space, Adaptivity, Polyhedral Functions, Convex Optimization

1 Introduction

The problem of solving linear systems subject to convex polyhedral constraints or subject to minimizing a convex polyhedral function arises in many applications. The most prominent examples of such problems are the minimization of $\|Au - f\|^2$ subject to linear inequality constraints $Bu \leq b$, or variational problems like the minimization of $\|u\|_1$ subject to $Au = f$. The latter has recently gained a lot of attention (particularly in compressed sensing and image processing) due to its desirable properties of enforcing sparsity. Further examples of polyhedral functions are $\|Tu\|_\infty$, and $\|Tu\|_1$ for any matrix T or the indicator function of equality constraints, inequality constraints, or the indicator function of a constraint restricting u to be in the convex hull of finitely many points.

In [BMBO11] we investigated the so called *inverse scale space flow* for solving problems of the form

$$J(u) \to \min_{u \in X} \qquad \text{subject to } Au = f, \tag{1.1}$$

and introduced a new and very efficient method for solving the above problem in the case of $J(u) = \|u\|_1$. In this paper we will generalize this method and prove that the underlying concept can be applied to any convex polyhedral function.

*Westfälische Wilhelms-Universität Münster, Institut für Numerische und Angewandte Mathematik, Einsteinstr. 62, D 48149 Münster, Germany (m.moeller@gmx.net, martin.burger@wwu.de)

The rest of the paper is organized as follows: In Section 2 we will briefly recall the main findings of [BMBO11] about the adaptive inverse scale space method (aISS). In the following Section 3 we will summarize the most important facts about polyhedral functions before we show in Section 4 how to generalize the aISS method to arbitrary polyhedral functions. We will analyze the convergence properties of our method in detail and prove finite time convergence. Furthermore, we will show in Section 5 that the popular (forward) scale space flow is the inverse scale space flow on the convex conjugate problem and can therefore also be solved with the aISS algorithm. In addition we show that the scale space flow is equivalent to a well known variational problem. In Section 6 we illustrate the concept of polyhedral functions and demonstrate the behavior of the aISS flow in several examples like problems with convex hull constraints, problems with linear inequality constraints or regularizations like $\|Tu\|_\infty$ or finding the best convex approximation of a noisy data set.

2 Inverse Scale Space Flows

2.1 Motivation for the inverse scale space flow

In this section we will recall the main results of [BMBO11]. For compressed sensing problems where the goal is to recover a sparse signal $u \in \mathbb{R}^n$ from measurements $f = Au$, $A \in \mathbb{R}^{m\times n}$, $m << n$, the Bregman iteration [OBGaY05, YOGD08] respectively its linearized version [COS09b, COS09a] have gained a lot of attention due to their efficiency and quality of the recovery results. The Bregman iteration constructs a sequence u_k as minimizers of

$$E_k(u) = \frac{\lambda}{2}\|Au - f\|^2 + J(u) - \langle p_{k-1}, u\rangle, \tag{2.1}$$

where p_{k-1} is an element of the subdifferential of a convex regularization functional J at u_{k-1}, $p_{k-1} \in \partial J(u_{k-1}) = \{p : J(u)-J(u_{k-1})-\langle p, u-u_{k-1}\rangle \geq 0 \ \forall u\}$. Each step is a penalized least squares problem with the (generalized) *Bregman distance*

$$D^{p_{k-1}}(u, u_{k-1}) = J(u) - J(u^k) - \langle p_{k-1}, u - u^k\rangle, \tag{2.2}$$

between u and u_{k-1} with respect to regularization function J. The optimality condition of (2.1) at the minimizer u_k is

$$p_k = p_{k-1} + \lambda A^*(f - Au_k) \in \partial J(u_k). \tag{2.3}$$

This equation can be interpreted as the implicit discretization of the time continuous equation

$$\partial_t p(t) = A^*(f - Au(t)), \qquad p(t) \in \partial J(u(t)), \tag{2.4}$$

which is called *inverse scale space method* and analyzed in [BGOX06].

2.2 The Adaptive Inverse Scale Space Method for ℓ^1 Regularitaion

One of the main findings of [BMBO11] was that for $J(u) = \|u\|_1$ problem (2.4) can be solved exactly without discretization due to the discrete nature of the time evolution of solutions. It has been shown that the solution $u(t)$ changes only at fixed times t_k, which can be calculated explicitly. This leads to an algorithm, called adaptive inverse scale space method (aISS), that converges in a finite number of iterations to the solution of the problem

$$\min_u \|u\|_1 \text{ such that } Au = f. \tag{2.5}$$

We can summarize the algorithm to achieve this as follows:

- Initialize $t_1 = \|A^T f\|_\infty$, $p(t_1) = t_1 A^T f$, $k = 1$
- repeat until $\|Au(t_k) - f\|^2 <$ threshold
  1. Calculate $u(t_k)$ as the minimizer of
  $$\|Au - f\|^2 \text{ subject to } p(t_k) \in \partial\|u\|_1 \tag{2.6}$$
  2. Determine the next time step by
  $$t_{k+1} = \min\{t \mid t > t_k, \exists j : |p_j(t)| = 1, u_j(t_k) = 0, p_j(t) \neq p_j(t_k)\}, \tag{2.7}$$
  where
  $$p_j(t) = p_j(t_k) + (t - t_k)e_j \cdot A^T(f - Au(t_k)) \tag{2.8}$$
  3. Update $p(t_k + 1)$ by Formula (2.8).
  4. $k \leftarrow k + 1$

For details on the method, the corresponding proof, and further convergence analysis we refer to [BMBO11]. The goal of this paper is to show how the above aISS concept generalizes to regularizations with polyhedral functions. Let us summarize the most important facts about polyhedral functions in the next section.

3 Convex polyhedral functions

We start with the general definitions of convex polyhedral functions and finitely generated convex functions from [Roc96]:

Definition 1. A function $J : \mathbb{R}^n \to R$ is called a polyhedral convex function if and only if J can be expressed in the form

$$J(u) = h(u) + \delta(u|C), \tag{3.1}$$

where

$$h(u) = \max_i\{\langle u, b_i\rangle - \beta_i \mid i \in 1, ..., k\}, \tag{3.2}$$

$$\delta(u|C) = \begin{cases} 0 & \text{if } u \in C, \\ \infty & \text{else ,} \end{cases} \tag{3.3}$$

$$C = \{u \mid \langle u, b_i\rangle \leq \beta_i \mid i \in k+1, ..., m\}. \tag{3.4}$$

Definition 2. A convex function $J : \mathbb{R}^n \to R$ is said to be finitely generated if there exist vectors $d_i \in R^n$, $i = 1, ..., m$, and corresponding scalars α_i such that

$$J(u) = \inf_{\{\lambda_i\}} \{\sum_{i=1}^{m} \lambda_i \alpha_i\}, \tag{3.5}$$

such that the infimum is taken over all λ_i for which

$$u = \sum_{i=1}^{m} \lambda_i d_i, \quad \sum_{i=1}^{l} \lambda_i = 1, \quad \lambda_i \geq 0 \ \ \forall i = 1, ..., m \tag{3.6}$$

Rockafellar proves that the definitions of "finitely generated" and "polyhedral" are equivalent for convex functions:

Lemma 1. *[Roc96]*
A convex function is polyhedral if and only if it is finitely generated. The infimum for a given u in the definition of "finitely generated convex functions" if finite, is attained by some choice of the coefficients λ_i.

Since the two definitions above are equivalent, we will from now on talk about the finitely generated fg-representation and the polyhedral p-representation of a convex polyhedral function. Moreover, the infimum in the definition of finitely generated is attained by some coefficients λ_i. Therefore, for a given polyhedral function in fg-representation, we can write any u as $u = \sum_{i=1}^{m} \lambda_i d_i$, $\sum_{i=1}^{l} \lambda_i = 1$, with coefficients $\lambda_i \geq 0$ such that $J(u) = \sum_{i=1}^{m} \lambda_i \alpha_i$. We will refer to this representation of u as the infimal coefficient ic-representation. Before we go into more details about polyhedral functions, let us look at a simple example:

Example 1. The function $J(u) = \|u\|_1$ is polyhedral. For simplicity, consider the 2d case. In the notation of the definition of polyhedral functions we can choose

$$b_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \ b_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, b_3 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, b_4 = \begin{pmatrix} -1 \\ -1 \end{pmatrix},$$
$$C = \mathbb{R}^2, \qquad \beta_i = 1 \ \forall i, \qquad k = 0$$

and easily see that indeed

$$\|u\|_1 = \max_i \langle b_i, u \rangle.$$

In the definition of finitely generated we have

$$d_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ d_2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, d_3 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, d_4 = \begin{pmatrix} 0 \\ -1 \end{pmatrix},$$
$$l = 0, \qquad \alpha_i = 1 \qquad \forall i.$$

It is interesting to see that the two representations of the $\|u\|_1$ norm have two geometric interpretations. In the p-representation the b_i are the normals of the unit ball of $\|u\|_1$ while in the fg-representation the ℓ^1 norm is expressed in terms of the edges of the unit normal ball. Thinking about the geometric relation between the primal and dual unit ball of a function it is not too surprising that the vectors in the fg-representation of the primal function become the vectors in the p-representation of the dual norm as the next theorem from [Roc96] shows.

Theorem 1. *[Roc96]*
The conjugate of a polyhedral convex function is polyhedral. More precisely, if a convex polyhedral function $J(u)$ is given in the fg-represention, using the notation from above, its convex conjugate is

$$\begin{aligned} J^*(p) &= h(p) + \delta(p|C), \\ h(p) &= \max_{i\in\{1,\dots,k\}} \{\langle d_i, p\rangle - \alpha_i\} \\ C &= \{p \mid \langle d_i, p\rangle \le \alpha_i \ \forall i \in \{k+1, ..., m\}\} \end{aligned} \tag{3.7}$$

We now know the connection between a polyhedral function and its convex conjugate. Since our goal is to derive a general inverse scale space algorithm for polyhedral functions, let us characterize the subdifferential of a polyhedral function in its fg-representation.

Lemma 2. *Let J be a convex finitely generated function in the notation of Definition 2. Then the subdifferential $\partial J(u)$ at $u = \sum_{i=1}^m \lambda_i d_i$ in ic-representation can be characterized as follows:*

$$p \in \partial J(u) \quad \Leftrightarrow \begin{cases} \langle p, d_i\rangle \le \alpha_i & \text{for } i \in \{l+1, ..., m\} \\ \lambda_i = 0 & \text{if } \langle p, d_i\rangle < \alpha_i \text{ for } i \in \{l+1, ..., m\} \\ \lambda_i = 0 & \text{if } i \notin I \end{cases} \tag{3.8}$$
$$I = \{1 \le i \le l \ : \ (\alpha_i - \langle p, d_i\rangle) = \min_k(\alpha_k - \langle p, d_k\rangle)\}$$

Proof. Let us prove the two implications of Lemma 2 separately.

- First, let us assume we have an element p which meets the three conditions on the right hand side of (3.8) for some u with ic-representation $u = \sum_{i=1}^m \lambda_i d_i$. We will show that $p \in \partial J(u)$. By definition $p \in \partial J(u)$ means

$$J(v) - J(u) - \langle p, v-u\rangle \ge 0 \qquad \forall v. \tag{3.9}$$

Let $v = \sum_{i=1}^{m} \nu_i d_i$ be an arbitrary element in ic-representation. Then

$$\begin{aligned}
& J(v) - J(u) - \langle p, v-u \rangle \\
= & \sum_{i=1}^{m} (\nu_i - \lambda_i)\big(\alpha_i - \langle p, d_i \rangle\big) \\
= & \sum_{i=1}^{l} (\nu_i - \lambda_i)\big(\alpha_i - \langle p, d_i \rangle\big) + \sum_{i=l+1}^{m} (\nu_i - \lambda_i) \underbrace{\big(\alpha_i - \langle p, d_i \rangle\big)}_{=0 \text{ if } \lambda_i > 0} \\
= & \sum_{i=1}^{l} (\nu_i - \lambda_i)\big(\alpha_i - \langle p, d_i \rangle\big) + \underbrace{\sum_{i=l+1, \lambda_i=0}^{m} \nu_i \big(\alpha_i - \langle p, d_i \rangle\big)}_{\geq 0} \\
\geq & \underbrace{\sum_{i=1}^{l} \nu_i \big(\alpha_i - \langle p, d_i \rangle\big)}_{\geq \min_k (\alpha_k - \langle p, d_k \rangle) \sum_{i=1}^{l} \nu_i} - \underbrace{\sum_{i=1}^{l} \lambda_i \big(\alpha_i - \langle p, d_i \rangle\big)}_{= \min_k (\alpha_k - \langle p, d_k \rangle) \sum_{i=1}^{l} \lambda_i} \\
\geq & \min_k \big(\alpha_k - \langle p, d_k \rangle\big) \underbrace{\Big(\sum_{i=1}^{l} \nu_i - \sum_{i=1}^{l} \lambda_i\Big)}_{=1-1=0} \\
= & 0
\end{aligned} \tag{3.10}$$

- Now let us assume the we have an element $u = \sum_{i=1}^{m} \lambda_i d_i$ in ic-represenation and $p \in \partial J(u)$. We need to show that the three conditions in the right hand side of (3.8) are satisfied.

  1. We prove the first inequality by contradiction. Assume that there exists a j with $\langle p, d_j \rangle > \alpha_j$. Let us define $v = \sum_{i=1}^{m} \nu_i d_i$ such that $\nu_i = \lambda_i$ for all $i \neq j$ and $\nu_j = \lambda_j + \epsilon$ with $\epsilon > 0$. Notice that we can not yet speak of this being the ic-representation of v since we have not shown that this choice of coefficients corresponds to the infimal choice as required in (3.5), but, since the ic-representation leads to the smallest energy among all such representations we know that $J(v) \leq \sum_i \nu_i \alpha_i$. Thus,

  $$\begin{aligned}
  & J(v) - J(u) - \langle p, v-u \rangle \\
  \leq & \sum_{i=1}^{m} (\nu_i - \lambda_i)\big(\alpha_i - \langle p, d_i \rangle\big) \\
  = & \epsilon \underbrace{\big(\alpha_j - \langle p, d_j \rangle\big)}_{<0 \text{ by assumption}} \\
  < & 0
  \end{aligned}$$

  This is a contradiction to $p \in \partial J(u)$, and therefore $\langle p, d_i \rangle \leq \alpha_i$ for $i \in \{l+1, ..., m\}$.

  2. For the second condition, we can use a similar argument as for the first. Assume there is a $j > l$ with $\langle p, d_j \rangle < \alpha_j$ but $\lambda_j > 0$. Again,

consider $v = \sum_{i=1}^{m} \nu_i d_i$ such that $\nu_i = \lambda_i$ for all $i \neq j$ and $\nu_j = 0$. Similar to the above we obtain

$$\begin{aligned} & J(v) - J(u) - \langle p, v-u \rangle \\ \leq \; & -\lambda_j \underbrace{\big(\alpha_j - \langle p, d_j \rangle\big)}_{>0 \text{ by assumption}} \\ < \; & 0, \end{aligned}$$

which again is a contradiction to $p \in \partial J(u)$. Therefore, $\lambda_i = 0$ if $\langle p, d_i \rangle < \alpha_i$ for $i \in \{l+1, ..., m\}$.

3. The last condition is also proved by contradiction. Let us assume that there is a $j \leq l$ for which $\lambda_j > 0$ although $(\alpha_j - \langle p, d_j \rangle) > \min_k(\alpha_k - \langle p, d_k \rangle)$. Now consider $v = \sum_{i=1}^{m} \nu_i d_i$ such that $\nu_i = \lambda_i$ for all $i \neq j$ and $i \neq c$, $\nu_j = 0$, $\nu_c = \lambda_c + \lambda_j$, where $c \in \arg\min_k(\alpha_k - \langle p, d_k \rangle)$. This way $\sum_{i=1}^{l} \nu_i = \sum_{i=1}^{l} \lambda_i = 1$, and therefore we can again argue that $J(v) \leq \sum_i \nu_i \alpha_i$ and compute

$$\begin{aligned} & J(v) - J(u) - \langle p, v-u \rangle \\ \leq \; & -\lambda_j \big(\alpha_j - \langle p, d_j \rangle\big) + (\nu_c - \lambda_c)\big(\alpha_c - \langle p, d_c \rangle\big) \\ = \; & \lambda_j \underbrace{\Big(\big(\alpha_c - \langle p, d_c \rangle\big) - \big(\alpha_j - \langle p, d_j \rangle\big)\Big)}_{<0} \\ < \; & 0. \end{aligned} \tag{3.11}$$

Again, the assumption led to a contradiction, which means that the third condition also holds and therefore concludes the proof.

□

Example 2. Let us look at our standard example $J(u) = \|u\|_1$ again. We know that in this case the d_i are the positive and negative unit normal vectors, $l = 0$, $\alpha_i = 1$, and $C = \mathbb{R}^n$. Thus, Lemma 2 tells us that for the representation $u = \sum_i \lambda_i d_i$ where $\sum \lambda_i \alpha_i$ is infimal, we have

$$p \in \partial J(u) \quad \Leftrightarrow \begin{cases} \langle p, d_i \rangle \leq 1 & \text{for } i \in \{1, ..., m\} \\ \lambda_i = 0 & \text{if } \langle p, d_i \rangle < 1 \text{ for } i \in \{1, ..., m\} \end{cases}$$

which, using our knowledge about the d_i, could be rewritten as

$$p \in \partial J(u) \quad \Leftrightarrow \begin{cases} \|p\|_\infty \leq 1 & \\ \lambda_i = 0 & \text{if } p_i < 1 \text{ for } i \in \{1, ..., m\} \end{cases}$$

and is a well known representation of the ℓ^1 subdifferential.

Similar to the adaptive inverse scale space method for ℓ^1 regularization, the adaptive inverse scale space method for polyhedral functions will first compute the subgradient p of some (unknown) element u and then find u in ic-representation by solving a low dimensional optimization problem. For this sake, it is important to classify the ic-represenations, because it is not obvious (and in general not true) that writing an element u as $u = \sum_i \lambda_i d_i$ automatically is an ic-representation. The following Lemma however classifies ic-representations in a way that easily allows to find the ic-representations of elements for a given subgradient.

Lemma 3. *Let $p \in \partial J(u)$. Then any representation of u as $u = \sum_{i=1}^m \nu_i d_i$, $\nu_i \geq 0$, $\sum_{i=1}^l \nu_i = 1$ for which*

$$\begin{cases} \nu_i = 0 & \text{if } \langle p, d_i \rangle < \alpha_i \text{ for } i \in \{l+1, ..., m\}, \\ \nu_i = 0 & \text{if } (\alpha_i - \langle p, d_i \rangle) > \min_k(\alpha_k - \langle p, d_k \rangle) \end{cases},$$

is an ic-representation of u.

Proof. Let $u = \sum_{i=1}^m \nu_i d_i$ be a representation of u that meets the above conditions and let $u = \sum_i \lambda_i d_i$ be an ic-representation of u, i.e. $J(u) = \sum_i \alpha_i \lambda_i$. Then

$$\begin{aligned} 0 &= \langle p, u - u \rangle \\ &= \sum_i \nu_i \langle p, d_i \rangle - \sum_i \lambda_i \langle p, d_i \rangle \end{aligned}$$

Because of $p \in \partial J(u)$ and Lemma 2 we know that $\langle p, d_i \rangle \leq \alpha_i$ for all $i > l$. Due to our assumptions above this means $\langle p, d_i \rangle = \alpha_i$ whenever $\nu_i > 0$ or $\lambda_i > 0$ for $i > l$. Therefore we can continue

$$\begin{aligned} 0 &= \sum_i \nu_i \langle p, d_i \rangle - \sum_i \lambda_i \langle p, d_i \rangle \\ &= \sum_{i=1}^l \nu_i \langle p, d_i \rangle + \sum_{i=l+1}^m \nu_i \alpha_i - \big(\sum_{i=1}^l \lambda_i \langle p, d_i \rangle + \sum_{i=l+1}^m \lambda_i \alpha_i \big) \\ &= \sum_{i=1}^l \nu_i (\langle p, d_i \rangle - \alpha_i) + \sum_{i=1}^m \nu_i \alpha_i - \big(\sum_{i=1}^l \lambda_i (\langle p, d_i \rangle - \alpha_i) + \sum_{i=1}^m \lambda_i \alpha_i \big) \\ &= \min_k(\alpha_k - \langle p, d_k \rangle) \sum_{i=1}^l -\nu_i + \sum_{i=1}^m \nu_i \alpha_i - \big(\min_k(\alpha_k - \langle p, d_k \rangle) \sum_{i=1}^l -\lambda_i + \sum_{i=1}^m \lambda_i \alpha_i \big) \\ &= -\min_k(\alpha_k - \langle p, d_k \rangle) + \sum_{i=1}^m \nu_i \alpha_i - \big(-\min_k(\alpha_k - \langle p, d_k \rangle) + \sum_{i=1}^m \lambda_i \alpha_i \big) \\ &= \sum_{i=1}^m \nu_i \alpha_i - \sum_{i=1}^m \lambda_i \alpha_i \end{aligned}$$

Therefore, $\sum_{i=1}^m \nu_i \alpha_i = \sum_{i=1}^m \lambda_i \alpha_i = J(u)$ and $\sum_{i=1}^m \nu_i d_i$ is an ic-representation of u. □

Example 3. Let us illustrate what the above lemma means in very simple example. Consider for $u \in \mathbb{R}$, $J(u) = |u| + \chi_{[-1,1]}(u)$, where $\chi_{[-1,1]}(u)$ is the characteristic function of $[-1, 1]$. The fg-represenation of J is $d_1 = -1$, $d_2 = 0$, $d_3 = 1$, $\alpha_1 = 1$, $\alpha_2 = 0$, $\alpha_3 = 1$, and $l = 3$. Let us look at some $0 < u < 1$. There are infinitely many ways to represent $u = \sum_{i=1} \lambda_i d_i$ with $\lambda_i \geq 0$, $\sum_i \lambda_i = 1$, however not all of them are ic-representations. In fact, in this example, the ic-representation is unique. The subgradient of $u > 0$ is $p = 1$ and we can use Lemma 3 to find an ic-representation. We have

$$\begin{aligned} \langle p, d_1 \rangle &= -1 < \alpha_1 \\ \langle p, d_2 \rangle &= 0 = \alpha_2 \\ \langle p, d_3 \rangle &= 1 = \alpha_3 \end{aligned}$$

Therefore, we have to choose $\lambda_1 = 0$ to obtain an ic-representation, which means $u = \lambda_2 d_2 + \lambda_3 d_3$ with $\lambda_2 = (1 - u)$ and $\lambda_3 = u$ is the ic-representation of u in our example.

We will see in the next section that an fg-representation of the regularizer is sufficient for an efficient adaptive inverse scale space flow algorithm. Before going into the details of this flow we need to mention that the fg-representation as defined in Definition 2 is not unique. Therefore, it makes sense to from now on only consider irredundant fg-representations.

Definition 3. An fg-representation of a convex polyhedral function is called irredundant if one can not discard any (d_i, α_i) without changing the function.

The irredundant fg-representation of a convex polyhedral function is unique (cf. [Sch87]).

4 The inverse scale space flow for an arbitrary polyhedral function

We will now develop an adaptive inverse scale space flow algorithm for solving

$$\min J(u) \qquad \text{such that} \quad u \in \arg \min_{J(u)<\infty} \|Au - f\|^2, \tag{4.1}$$

where $J(u)$ is a given convex polyhedral function in fg-representation. Opposed to the ℓ^1 inverse scale space flow from [BMBO11], we have to pay a little more attention to the starting point $u_0 = u(0), p_0 = p(0)$ of the flow, since $(0, 0)$ no longer needs to satisfy $p_0 \in \partial J(u_0)$. In the next subsection we will first prove that the inverse scale space flow for any polyhedral function has a piecewise constant solution, before, in the following subsection, discussing how to find an appropriate starting point.

4.1 Generalized aISS flow algorithm

We will now show that the inverse scale space flow

$$\partial_t p(t) = A^T(f - Au(t)) \qquad p(t) \in \partial J(u(t)), \tag{4.2}$$

has a piecewise constant solution for any convex polyhedral $J(u)$ and that the solution can be calculated without any discretization of the above equation. All we need is a starting point $(p_0, u_0) = (p(0), u(0))$ such that

$$u_0 = \arg \min_u \|Au - f\|^2 \qquad \text{such that } p_0 \in \partial J(u_0). \tag{4.3}$$

We will discuss how to obtain such a starting point and what influence it has on the flow in detail in the next subsection. Let us first state the result of a piecewise constant flow:

Theorem 2. *There exists a sequence of times*

$$0 = t_0 < t_1 < t_2 < \dots$$

such that

$$u(t) = u(t_k), \qquad p(t) = p(t_k) + (t - t_k)A^T(f - Au(t_k)) \tag{4.4}$$

for $t \in [t_k, t_{k+1})$ *is a solution of the inverse scale space flow* (4.2) *with starting point* (p_0, u_0) *satisfying* (4.3)*, where* $u(t_k)$ *is a solution of*

$$\|Au - f\| \to \min_{u, p(t_k) \in \partial J(u)}. \tag{4.5}$$

Proof. By the assumption on our starting point, $u(t_0)$ satisfies (4.5). Now we proceed inductively to show that (4.4) is a solution to (4.2) for $t \in [t_k, t_{k+1})$, $t_{k+1} > t_k$. Given $p(t_k)$, we define

$$\begin{aligned} I_1(t) &= \{1 \le i \le l \ : \ (\alpha_i - \langle p(t), d_i\rangle) = \min_j(\alpha_j - \langle p(t), d_j\rangle)\}, &(4.6)\\ I_2(t) &= \{l+1 \le i \le m \ : \ \alpha_i = \langle p(t), d_i\rangle\}, &(4.7)\end{aligned}$$

for $p(t)$ defined by (4.4). Our goal is to show that $p(t) \in \partial J(u(t_k))$ holds for some $t > t_k$. By the characterization of the subdifferential (Lemma 2), this is the case if we can verify the following four criteria

- For $i \in \{1, ...l\}$, $i \notin I_1(t_k)$, $\Rightarrow i \notin I_1(t)$ for some $t > t_k$.
- For $i \in \{l+1, ...m\}$, $i \notin I_2(t_k)$, $\Rightarrow i \notin I_2(t)$ for some $t > t_k$.
- For $i \in I_1(t_k)$, $\Rightarrow i$ remains in $I_1(t)$ for some $t > t_k$, or $(\alpha_i - \langle p(t), d_i\rangle) \ge \min_j(\alpha_j - \langle p(t), d_j\rangle)$ and $\lambda_i = 0$ in the ic-representation of $u(t_k)$.
- For $i \in I_2(t_k)$, $\Rightarrow i$ remains in $I_2(t)$ for some $t > t_k$, or $\langle p(t), d_i\rangle \le \alpha_i$ and $\lambda_i = 0$ in the ic-representation of $u(t_k)$.

Notice that $u(t_k)$ minimizes $\|Au - f\|$ subject to the constraint $p(t_k) \in \partial J(u(t_k))$. By the characterization of the subdifferential (Lemma 2) we can conclude that $u(t_k)$ has an ic-representation $u(t_k) = \sum \lambda_i^k d_i = D\lambda$ which is the solution to the optimization problem

$$\min_\lambda \|AD\lambda - f\|^2$$
$$\text{such that } \lambda_i \ge 0,\ \sum_{i=1}^l \lambda_i = 1,\ \lambda_i = 0 \text{ if } i \notin I_1(t_k),\ \lambda_i = 0 \text{ if } i \notin I_2(t_k)$$

Notice that by Lemma 3 we know that any set $\{\lambda_i\}$ determined by the above minimization automatically yields an ic-representation of $u(t^k)$. We will discuss the situation for four cases separately.

- For $i \in \{1, ...l\}$, $i \notin I_1(t_k)$ we have $\lambda_i = 0$ and

  $$(\alpha_i - \langle p(t_k), d_i\rangle) > \min_j(\alpha_j - \langle p(t_k), d_j\rangle).$$

  Therefore, for $p(t)$ defined by (4.4),

  $$(\alpha_i - \langle p(t), d_i\rangle) > \min_j(\alpha_j - \langle p(t), d_j\rangle)$$

  holds for some $t > t^k$ small enough.

- For $i \in \{l+1, ...m\}$, $i \notin I_2(t_k)$ we have $\lambda_i = 0$ and

$$\langle p(t_k), d_i \rangle < \alpha_i.$$

Therefore, for $p(t)$ defined by (4.4),

$$\langle p(t), d_i \rangle < \alpha_i.$$

holds for some $t > t^k$ small enough.

- For $i \in I_2(t_k)$ the optimality conditions to (4.8) allow us to conclude that

$$\langle d_i, A^T(f - Au) \rangle = c_i, \tag{4.8}$$

for some Lagrange multiplier $c_i \leq 0$, which enforces the non-negativity of λ_i. There are two cases:

  1. Either $\lambda_i = 0$. In this case $\langle d_i, A^T(f - Au(t_k)) \rangle \leq 0$ and therefore

  $$\langle d_i, p(t) \rangle \leq \langle d_i, p(t_k) \rangle = \alpha_i,$$

  for any $t \geq t_k$.

  2. Or $\lambda_i > 0$. In this case the complimentary slackness condition tells us that $c_i = 0$ and therefore

  $$\langle d_i, p(t) \rangle = \langle d_i, p(t_k) \rangle = \alpha_i,$$

  which means $i \in I(t)$ for any $t \geq t_k$.

In either case we have either have $i \in I(t)$ or $\langle d_i, p(t) \rangle \leq \alpha_i$ and $\lambda_i = 0$ for any $t \geq t_k$.

- For $i \in I_1(t_k)$ the optimality conditions to (4.8) allow us to conclude that

$$\langle d_i, A^T(f - Au) \rangle = c_i + \beta,$$

for some Lagrange multiplier $c_i \leq 0$, which enforces the non-negativity of λ_i and another multiplier β shared by all λ_i with $i \in \{1, ...l\}$, which enforces the sum to one constraint. Similar to the previous point we can distinguish between two cases:

  1. Either $\lambda_i > 0$, which by complementary slackness means that $c_i = 0$ and

  $$\begin{aligned}(\alpha_i - \langle d_i, p(t) \rangle) &= (\alpha_i - \langle d_i, p(t_k) \rangle) - (t - t_k)\beta \\ &= \min_j(\alpha_j - \langle d_j, p(t_k) \rangle) - (t - t_k)\beta \end{aligned} \tag{4.9}$$

  2. Or $\lambda_i = 0$, which means that

  $$\begin{aligned}(\alpha_i - \langle d_i, p(t) \rangle) &= (\alpha_i - \langle d_i, p(t_k) \rangle) - (t - t_k)(c_i + \beta) \\ &\geq (\alpha_i - \langle d_i, p(t_k) \rangle) - (t - t_k)\beta \end{aligned} \tag{4.10}$$

Therefore, either $(\alpha_i - \langle d_i, p(t) \rangle)$ evolves in time by subtracting $(t - t_k)\beta$ from the previous minimum, or $\lambda_i = 0$ and $(\alpha_i - \langle d_i, p(t) \rangle)$ is as most as small as $(\alpha_i - \langle d_i, p(t_k) \rangle) - (t - t_k)\beta$ possibly making this index leave $I_1(t)$.

The above case study shows that there exists a time $t > t_k$ for which $p(t) \in \partial J(u(t_k))$. The time where the solution changes, can be calculated as the minimal time at which a new coefficient enters $I_1(t)$ or $I_2(t)$, i.e.

$$t_{k+1} = \min \left\{ \{t > t_k \mid \exists i \in I_1(t), i \notin I_1(t_k)\} \cup \{t > t_k \mid \exists i \in I_2(t), i \notin I_2(t_k)\} \right\} \tag{4.11}$$

If the above set in which we want to find the minimal t is empty, it obviously means that $p(t) \in \partial J(t(t^k))$ for all $t \geq t^k$. The flow has reached a stationary solution and we define $t^{k+1} = \infty$. Otherwise, by continuity of $p(t)$ we obtain

$$p(t_{k+1}) = p(t_k) + (t_{k+1} - t_k) \cdot A^T(f - Au(t_k)), \tag{4.12}$$

and can determine the next solution $u(t_{k+1})$ by solving the next optimization problem. The existence of a solution to (4.5) follows from standard convex optimization/quadratic programming arguments. □

Proposition 1. *The time step in* (4.11) *can be determined by*

$$t^{k+1} = \min(T_1 \cup T_2) \tag{4.13}$$

for the two sets

$$\begin{aligned} T_1 &= \{t_i \mid i \in \{1,..,l\}, i \notin I_1(t^k), t_i = t^k + \frac{(\alpha_i - \alpha_j) - \langle p(t^k), d_i - d_j \rangle}{\langle A^T(f - Au(t^k)), d_i - d_j \rangle}\} \\ T_2 &= \{t_i \mid i \in \{l+1,..,m\}, i \notin I_2(t^k), t_i = t^k + \frac{\alpha_i - \langle p(t_k), d_i \rangle}{\langle A^T(f - Au(t^k)), d_i \rangle}\} \end{aligned}$$

where in the definition of T_1, j is any index $j \in I_1(t^k)$ such that $\lambda_j > 0$. Due to the $\sum_{i=1}^{l} \lambda_i = 1$ constraint, such an index has to exist.

Proof. The above formulas follow from the equations $\alpha_i - \langle p(t_i), d_i \rangle = \alpha_j - \langle p(t_i), d_j \rangle$ and $\alpha_i = \langle p(t_i), d_i \rangle$ with $p(t)$ as defined in (4.4). □

The above Theorem and Proposition imply an algorithm to compute the exact solution to the inverse scale space flow for polyhedral functions, which is given as Algorithm 1 below.

Algorithm 1 Adaptive Inverse Scale Space Method for Polyhedral Functions

1. **Parameters:** A, f, threshold ≥ 0
2. **Initialization:** Find a starting point for which (4.3) is satisfied (also see Section 4.2).

while $\|Au(t_k) - f\| >$ threshold **do**

Find next time step t^{k+1} according to Proposition 1.
Compute $p(t^{k+1})$ and update $I_1(t^{k+1})$ and $I_2(t^{k+1})$ accordingly.
Let $I = I_1(t^{k+1}) \cup I_2(t^{k+1})$. Compute $u(t_{k+1}) = D\lambda$ via

$$\lambda = \arg\min_{\lambda} \left\{ \|ADP_I\lambda - f\|^2 \right\} \text{ subject to } \lambda \geq 0, \sum_{i \in I_1(t^k+1)} \lambda_i = 1. \tag{4.14}$$

Here D denotes the matrix whose columns are the d_i and P_I is a projection onto the index set I.

end while
return $u(t_k)$

We have seen that the inverse scale space flow stays piecewise constant and its solution can be calculated easily. Once a starting point is found, each step only contains of finding the minimal time t^{k+1}, updating $p(t^{k+1})$, $I_1(t^{k+1})$ and $I_2(t^{k+1})$ explicitly and solving a least squares problem with a sum to one constraint for the index set $I_1(t^{k+1})$. Notice that aISS is very efficient if the solution has a sparse representation in the d_i, since in this case the optimization problem becomes very low dimensional.

In the next subsection, we will go into more details about how to find a starting point.

4.2 Starting point of the aISS flow

As a starting point for the aISS flow we need a p_0 and corresponding u_0 such that (4.3) holds. Therefore, we have to find a solution to the inequalities

$$\langle d_i, p\rangle \leq \alpha_i \qquad \forall i \in \{l+1, ..., m\}. \tag{4.15}$$

For reasons to be discussed later the additional condition $p_0 \in \text{range}(A^T)$ sometimes is desirable, which would modify the problem to finding a solution q_0 to the inequalities

$$\langle Ad_i, q\rangle \leq \alpha_i \qquad \forall i \in \{l+1, ..., m\}, \tag{4.16}$$

and setting $p_0 = A^T q_0$. Once a p_0 is found the corresponding u_0 can be found by solving the optimization problem (4.3). This optimization problem becomes a non-negative least squares problem for the λ_i in the ic-representation of u_0, where only those λ_i are non-zero for which

$$\langle d_i, p_0\rangle = \alpha_i \qquad i \in \{l+1, ..., m\} \tag{4.17}$$

$$\alpha_i - \langle d_i, p_0\rangle = \min_{k\in\{1,...,l\}} \alpha_k - \langle d_k, p_0\rangle \qquad i \in \{1, ..., l\} \tag{4.18}$$

Thus, since we should assume a sparse ic-representation of final solution u in the λ_i, it makes sense to try to choose p_0 such that the above index sets are as small as possible. Let us investigate a special type of polyhedral functions $J(u)$ in more detail:

Lemma 4. *Let J be given in its irredundant fg-representation. If $J(u) \geq 0$ and $J(u) = 0$ if and only if $u = 0$, then $\alpha_i > 0$ $\forall i > l$ and if $l > 0$ there is a $j \leq l$ such that $d_j = 0$, $\alpha_j = 0$ and $\alpha_i > 0$ $\forall i \neq j$.*

Proof. For $d_i \neq 0$ we have $0 < J(d_i) = \inf_{d_i = \sum_j \lambda_j d_j} \sum_j \lambda_j d_j \leq \alpha_i$. If $l > 0$ there is a representation $0 = \sum_i \lambda_i d_i$ such that $\sum_{i=1}^{l} \lambda_i = 1$ and $0 = J(0) = \sum_i \lambda_i \alpha_i$. As seen above, $\alpha_i > 0$ for any i corresponding to a $d_i \neq 0$. Due to the constraint $\sum_{i=1}^{l} \lambda_i = 1$ at least one λ_j $j \leq l$ has to be greater than zero. Since both α_i and λ_i have to be greater or equal to zero, $0 = \sum_i \lambda_i \alpha_i$ is only possible for $\alpha_j = 0$ and $d_j = 0$. □

Conclusion 1. *If $J(u) \geq 0$ and $J(u) = 0$ if and only if $u = 0$, then*

$$0 = \arg \min_{0 \in \partial J(u)} \|Au - f\|^2, \tag{4.19}$$

or in other words, $u_0 = 0$, $p_0 = 0$ is a consistent starting point for aISS.

Proof. According to Lemma 4 $\alpha_i > 0$ except for one α_j corresponding to $d_j = 0$ (if $l > 0$). Therefore, $\langle d_i, 0\rangle < \alpha_i$ for all $i > l$, and thus all corresponding λ_i are zero. For $i \le l$ the minimum of all $(\alpha_i - \langle d_i, 0\rangle)$ is attained at $i = j$ and thus the only valid ic-representation of a u_0 for which $p_0 \in \partial J(u_0)$ is $u_0 = d_j = 0$. $\square$

We have established $u_0 = 0$, $p_0 = 0$, as a consistent starting point for the aISS flow if J has the property $J(u) \ge 0$ with equality only for $u = 0$, which already covers a wide variety of regularizers. One popular class of functions not covered by the above analysis are indicator functions of polyhedral sets, like e.g. non-negativity constraints or, more generally, constraints of the form $Bu \le b$. Let us assume $u = 0$ meets the $Bu \le b$ constraint, i.e. $b \ge 0$. Many problems can at least be expressed as a translation of this setting. Since indicator functions map onto $\{0, \infty\}$, the α_i for all valid points are zero. Although this again makes $p_0 = 0$ a valid starting subgradient, this is not a good choice since $\alpha_i - \langle d_i, p_0\rangle = 0$ for all i and thus the solution is completely dense in its ic-representation.

If the set described by $Bu \le b$ is bounded, then $l = m$ and we suggest to choose $p_0 = d_j$ for a d_j which has maximal norm, since in this case $\alpha_j - \langle d_j, p_0\rangle = -\|d_j\|^2$ is the unique minimum and u_0 is 1-sparse with only λ_j possibly being non-zero. If $l < m$ the situation is more complicated and one should try to find a p_0 such that the minimum $\min_{i \le l} \alpha_i - \langle d_i, p_0\rangle$ is attained at as few indices as possible, while $\alpha_i > \langle d_i, p_0\rangle$ holds for as many indices $i > l$ as possible. This choice guarantees a sparse starting point.

4.3 Convergence

As we have seen in the previous two subsections, choosing a starting point will be easy in most cases and with an appropriate starting point the piecewise constant solution to the aISS flow can be computed efficiently. In this subsection we will establish some convergence properties of the flow. Let us start with the strict decrease of the approximation to f at each time step:

Proposition 2. *The approximation error $\|Au(t) - f\|$ of the inverse scale space flow for polyhedral functions is strictly decreasing at the times t_k, i.e.*

$$\|Au(t_{k+1}) - f\| < \|Au(t_k) - f\| \tag{4.20}$$

Proof. We will prove the above Proposition in two steps

1. Show that $\|Au(t_{k+1}) - f\| < \|Au(t_k) - f\|$ if $p(t_k) \notin \partial J(u(t_{k+1}))$.
2. Show that $p(t_k) \notin \partial J(u(t_{k+1}))$ is always satisfied.

First part: Let us assume that $p(t_k) \notin \partial J(u(t_{k+1}))$. In this case

$$D^{p(t_k)}(u(t_{k+1}), u(t_k)) > 0. \tag{4.21}$$

Notice that $u(t_{k+1})$ is a minimizer of

$$Q(u) = \frac{1}{2}(t_{k+1} - t_k)\|Au - f\|^2 + D^{p(t_k)}(u, u(t_k)), \tag{4.22}$$

which can easily be verified by confirming that the formula for $p(t_{k+1})$ coincides with the optimality condition of the above functional. Using (4.21) this yields the conclusion

$$\begin{aligned}\frac{1}{2}(t_{k+1}-t_k)\|Au(t_{k+1})-f\|^2 &< Q(u(t_{k+1}))\\ &\leq Q(u(t_k))\\ &= \frac{1}{2}(t_{k+1}-t_k)\|Au(t_k)-f\|^2,\end{aligned}$$

and since $(t_{k+1}-t_k)>0$ we have shown $\|Au(t_{k+1})-f\|<\|Au(t_k)-f\|$.

Second part: By construction, more specific by the choice of t^{k+1}, there exists an index i such that $i\in I_1(t_{k+1})$, $i\notin I_1(t_k)$ or $i\in I_2(t_{k+1})$, $i\notin I_2(t_k)$. By the characterization of the subdifferential of $J(u)$, we have to have $\lambda_i=0$ in the ic-representation of $u(t_{k+1})$, because otherwise $i\notin I_1(t_k)$, (respectively $i\notin I_2(t_k)$), implies $p(t_k)\notin\partial J(u(t_{k+1}))$ and we are done. If all $\lambda_i=0$ at the indices that newly entered $I_1(t_{k+1})$ or $I_2(t_{k+1})$, then we can conclude that $u(t_{k+1})=u(t_k)$ since the remaining λ_j in the ic-representation of $u(t_{k+1})$ solve the same optimization problem as they did for $u(t_k)$. However, we will show that the assumption $u(t_{k+1})=u(t_k)$ leads to a contradiction:

1. If there exists an $i\in I_2(t_{k+1})$, $i\notin I_2(t_k)$, and $u(t_{k+1})=u(t_k)$ then

$$\begin{aligned}\alpha_i &\overset{i\in I_2(t_{k+1})}{=} \langle d_i,p(t_{k+1})\rangle\\ &= \langle d_i,p(t_k)\rangle+(t_{k+1}-t_k)\langle d_i,A^T(f-Au(t_k))\rangle\\ &= \underbrace{\langle d_i,p(t_k)\rangle}_{<\alpha_i,\text{ since } i\notin I_2(t_k)} +(t_{k+1}-t_k)\underbrace{\langle d_i,A^T(f-Au(t_{k+1}))\rangle}_{\leq 0 (\text{compare } (4.8))}\\ &< \alpha_i\end{aligned}$$

2. If there exists an $i\in I_1(t_{k+1})$, $i\notin I_1(t_k)$, and $u(t_{k+1})=u(t_k)$ then

$$\begin{aligned}(\alpha_i-\langle d_i,p(t_{k+1})\rangle) &\overset{i\in I(t_{k+1})}{=} \min_j(\alpha_j-\langle d_j,p(t_{k+1})\rangle)\\ &\overset{\text{compare } (4.9)}{=} \min_j(\alpha_j-\langle d_j,p(t_k)\rangle)-(t_{k+1}-t_k)\beta\\ &\overset{i\notin I(t_{k+1})}{<} (\alpha_i-\langle d_i,p(t_k)\rangle)-(t_{k+1}-t_k)\beta\\ &\overset{compare (4.10)}{\leq} (\alpha_i-\langle d_i,p(t_{k+1})\rangle)\end{aligned}$$

□

The previous proposition allows us to conclude the finite time convergence of the aISS method:

Theorem 3. *Let $(u(t),p(t))$ be a solution of the adaptive inverse scale space method as above, then there exists a $K>0$ such that $t_{K+1}=\infty$.*

Proof. If there existed a $k\neq j$ such that $I_1(t_k)=I_1(t_j)$ and $I_2(t_k)=I_2(t_j)$ then we would obviously have $u(t_k)=u(t_j)$ and therefore $\|Au(t_k)-f\|^2=$

$\|Au(t_j) - f\|^2$. By Proposition 2 this is impossible. Since in finite dimensions there are only finitely many possibilities for indices to be (or not to be) in $I_1(t_k)$ and $I_2(t_k)$, we can conclude that the method has to converge in a finite number of iterations, i.e. there exists a $K > 0$ such that $t_{k+1} = \infty$. □

In the previous literature on Bregman iterations and inverse scale space methods it has been shown already that the solution $u(t)$ of the inverse scale space flow converges to a J-minimizing solution of $Au = f$ or, if $f \notin \text{range}(A)$, to a J-minimizing solution such that $u \in \arg\min \|Au - f\|^2$. However, different from the previous literature, our starting point does not have to be $(0, 0)$. Furthermore, we allow $J(u) = \infty$ which might lead to the case where $f \in \text{range}(A)$, but for any solution to $Au = f$ we have $J(u) = \infty$. Both aspects are not covered by the previous analysis. Let us start with a lemma similar to Proposition 3.2 in [OBGaY05].

Lemma 5. *The inverse scale space flow for polyhedral norms meets*

$$\begin{aligned} & D^{p(t^{k+1})}(u, u(t^k)) - D^{p(t^k)}(u, u(t^{k-1})) \\ \leq \ & \frac{(t^{k+1} - t^k)}{2} \left(\|Au - f\|^2 - \|Au(t^k) - f\|^2 \right) \end{aligned} \tag{4.23}$$

for all u for which $J(u) \leq \infty$

Proof. First of all notice, that the inverse scale space flow has the interesting property of $p(t^k) \in \partial J(u(t^k))$ as well as $p(t^k) \in \partial J(u(t^{k-1}))$, such that $D^{p(t^k)}(u(t^k), u(t^{k-1})) = 0$ for all k. We can calculate

$$\begin{aligned} & D^{p(t^{k+1})}(u, u(t^k)) - D^{p(t^k)}(u, u(t^{k-1})) \\ = \ & D^{p(t^{k+1})}(u, u(t^k)) + D^{p(t^k)}(u(t^k), u(t^{k-1})) - D^{p(t^k)}(u, u(t^{k-1})) \\ = \ & \langle u(t^k) - u, p(t^{k+1}) - p(t^k), \rangle \\ = \ & (t^{k+1} - t^k) \langle u(t^k) - u, A^T (f - Au(t^k)), \rangle \\ \leq \ & \frac{(t^{k+1} - t^k)}{2} \left(\|Au - f\|^2 - \|Au(t^k) - f\|^2 \right), \end{aligned}$$

where the last step comes from $2A^T(Au(t^k) - f)$ being in the subdifferential of $\|Au - f\|^2$ at $u(t^k)$. □

We can use the above lemma to state the following convergence result:

Theorem 4. $t_{K+1} = \infty$ *if and only if* $u(t_K) \in \arg\min_{J(u)<\infty} \|Au - f\|^2$. *More precisely, for any* $\tilde{u} \in \arg\min_{J(u)<\infty} \|Au - f\|^2$ *we have*

$$\|Au(t^k) - f\|^2 \leq \|A\tilde{u} - f\|^2 + \frac{2D^{p_0}(\tilde{u}, u_0)}{t^{k+1}}. \tag{4.24}$$

for any k.

Proof. Let us start with proving the estimate (4.24). We sum over estimate

(4.23) yielding the left hand side

$$
\begin{aligned}
&\sum_{i=1}^{k}\Big(D^{p(t^{i+1})}(u,u(t^i)) - D^{p(t^i)}(u,u(t^{i-1}))\Big)\\
= \quad & D^{p(t^{k+1})}(u,u(t^k)) - D^{p(t^1)}(u,u(t^0)),\\
\geq \quad & -\big(J(u) - J(u(t^0)) - \langle p(t^1), u-u(t^0)\rangle\big),\\
= \quad & -D^{p(t^0)}(u,u(t^0)) - (t^1-t^0)\langle A^T(Au(t^0)-f), u(t^0)-u\rangle,\\
\geq \quad & -D^{p(t^0)}(u,u(t^0)) - \frac{(t^1-t^0)}{2}\big(\|Au(t^0)-f\|^2 - \|Au-f\|^2\big).
\end{aligned}
$$

For the right hand side we use the monotone decay of $\|Au(t^i)-f\|^2$ (Proposition 2) to obtain

$$
\begin{aligned}
&\sum_{i=1}^{k}\frac{(t^{i+1}-t^i)}{2}\big(\|Au-f\|^2 - \|Au(t^i)-f\|^2\big)\\
\leq \quad & (\|Au-f\|^2 - \|Au(t^k)-f\|^2)\sum_{i=1}^{k}\frac{(t^{i+1}-t^i)}{2},\\
= \quad & \frac{t^{k+1}-t^1}{2}(\|Au-f\|^2 - \|Au(t^k)-f\|^2),
\end{aligned}
\tag{4.25}
$$

Reading the full estimate we have

$$
\begin{aligned}
&\frac{t^{k+1}-t^1}{2}(\|Au-f\|^2 - \|Au(t^k)-f\|^2)\\
\geq \quad & -D^{p(t^0)}(u,u(t^0)) - \frac{(t^1-t^0)}{2}(\|Au(t^0)-f\|^2 - \|Au-f\|^2)
\end{aligned}
\tag{4.26}
$$

which is equivalent to (4.24) and holds for any u with $J(u) < \infty$.

As for the equivalence:

- $t^{K+1} < \infty$ while $u(t^K) \in \arg\min_{J(u)<\infty}\|Au-f\|^2$ would contradict Proposition 2
- By the estimate we just showed, $t^{K+1} = \infty$ means $\|Au(t^K)-f\|^2 \leq \|Au-f\|^2$ for all u with $J(u) < \infty$ and thus $u(t^K) \in \arg\min_{J(u)<\infty}\|Au-f\|^2$.

□

Lemma 6. *For a convex set $\{u \mid J(u) < \infty\}$ and M defined by*

$$
M = \{u \mid u \in \arg\min_{J(u)<\infty}\|Au-f\|^2\} \tag{4.27}
$$

the set

$$
\{Au \mid u \in M\} \tag{4.28}
$$

consists of only one element (unless $J(u) \equiv \infty$).

Proof. The elements in $\{Au \mid u \in M\}$ are the solutions of

$$\min_{q \in C} \|q - f\|^2$$

with $C = \{Au \mid J(u) < \infty\}$. For a convex polyhedral J, C is non-empty, closed and convex. Since the ℓ^2 norm is strictly convex, the above minimizer is unique. □

Theorem 5. *The stationary solution $u(t_K)$ of the inverse scale space flow with starting point p_0 minimizes the Bregman distance*

$$D^{p_0}(u, u_0) = J(u) - J(u_0) - \langle p_0, u - u_0 \rangle, \tag{4.29}$$

among all $u \in \arg\min_{J(u)<\infty} \|Au - f\|^2$. In particular, if $p_0 \in range(A^T)$ then $u(t_K)$ is $J(u)$-minimizing.

Proof. Let u be any $u \in \arg\min_{J(u)<\infty} \|Au - f\|^2$. Since $p(t_K) \in \partial J(u(t_K))$ we know that

$$\begin{aligned}
0 &\leq D^{p(t_K)}(u, u(t_K)) \\
&= J(u) - J(u(t_K)) - \big\langle p(t_K), u - u(t_K) \big\rangle \\
&= J(u) - J(u(t_K)) - \big\langle p(0) + \sum_{i=1}^{K} (t_i - t_{i-1}) A^T (f - Au(t_{i-1})), u - u(t_K) \big\rangle \\
&= J(u) - J(u(t_K)) - \big\langle p(0), u - u(t_K) \big\rangle \\
&\quad - \big\langle \sum_{i=1}^{K} (t_i - t_{i-1})(f - Au(t_{i-1})), \underbrace{Au - Au(t_K)}_{=0 \text{ due to Lemma 6}} \big\rangle \\
&= J(u) - J(u(t_K)) - \big\langle p(0), u - u(t_K) \big\rangle,
\end{aligned} \tag{4.30}$$

Rearranging this inequality and extending with u_0 leads to

$$\begin{aligned}
J(u(t_K)) - J(u_0) - \langle p_0, u(t_K) - u_0 &\leq J(u) - J(u_0) - \big\langle p(0), u - u_0 \big\rangle, \\
\Rightarrow D^{p_0}(u(t_K), u_0) \leq D^{p_0}(u, u_0)
\end{aligned} \tag{4.31}$$

for all $u \in \arg\min_{J(u)<\infty} \|Au - f\|^2$. □

Notice that above theorem allows us to incorporate a-priori information into the solution of our problem. If we for instance know that a certain coefficient λ_i, $i > l$, in the ic-representation of the true solution is likely to be non-zero we could choose a p_0 such that $\langle p_0, d_i \rangle = \alpha_i$, which would basically lead to not penalizing this particular coefficient. Of course, care has to be taken when incorporating such prior knowledge since choosing a $p_0 \notin \text{range}(A^T)$ based on false a-priori assumptions can lead to weakening the performance of the regularization J.

So far, we have seen the strict decay of $\|Au - f\|$ at each time step, concluded the finite time convergence and seen that the final solution of the aISS method is J-minimizing among all $u \in \arg\min_{J(u)<\infty} \|Au - f\|^2$, if $p_0 \in \text{range}(A^T)$. As seen earlier, $p_0 = 0$ is a valid starting point for $J(u)$ with $J(u) \geq 0$ and $J(u) = 0 \Leftrightarrow u = 0$. For this starting point $p_0 \in \text{range}(A^T)$ automatically holds. For indicator functions, the starting point is less obvious to choose, but also less important, since we are just looking for one possible $u \in \arg\min_{J(u)<\infty} \|Au - f\|^2$:

Conclusion 2. *For indicator functions $J(u)$ the condition $p_0 \in range(A^T)$ is not crucial. Being able to possibly determine different Bregman distance minimizing solutions to $u \in \arg\min_{J(u)<\infty} \|Au - f\|^2$ simply reflects possible non-uniqueness of the minimizer.*

Finally, we can state the exact recovery of very special $f = Au_{\text{true}}$ as well as a result about the d_i being eigenfunctions, if A is normalized in a certain way.

Proposition 3. *Let $u_0 = 0$, $p_0 = 0$ be a valid starting point and let the data f be $f = \gamma Ad_i$, $\gamma > 0$. If the matrix A is normalized such that*

$$\alpha_j \|Ad_i\|^2 \geq \alpha_i \langle Ad_i, Ad_j \rangle, \tag{4.32}$$

then aISS converges in a single iteration. Furthermore, if the above inequality is strict, then $u(t_1) = \gamma d_i$.

Proof. In the aISS flow we have $p(t) = tA^T f = t\gamma A^T Ad_i$ and t^1 being the smallest time among all t_j at which

$$\begin{aligned} \alpha_j &= \langle p(t_j), d_j \rangle \\ \Rightarrow \quad t_j &= \frac{\alpha_j}{\gamma \langle d_j, d_i \rangle}. \end{aligned} \tag{4.33}$$

Thus, λ_i is allowed to be non-zero at t^1 if $t_i \leq t_j$, i.e. if

$$\begin{aligned} \frac{\alpha_i}{\gamma \langle d_i, d_i \rangle} &\leq \frac{\alpha_j}{\gamma \langle d_j, d_i \rangle}, \\ \Leftrightarrow \quad \alpha_j \|Ad_i\|^2 &\geq \alpha_i \langle Ad_i, Ad_j \rangle. \end{aligned} \tag{4.34}$$

If this is the case $\min_{p(t^1) \in \partial J(u)} \|Au - f\|^2 = 0$ and thus aISS converges in one step. If the above inequality is strict, then λ_i is the only non-zero coefficient in the ic-representation of $u(t^1)$ and therefore $u(t^1) = \gamma d_i$. ☐

In [Ben] Benning introduced/generalized the concept of eigenfunctions for quadratic minimization problems with respect to general regularizers $J(u)$ as function for which there exists a $\lambda > 0$ such that

$$\lambda A^T Au \in \partial J(u)$$

This idea will be extended by Benning and Burger in [BB]. We can show that for polyhedral functions the d_i correspond to eigenfunctions if the matrix A meets a certain normalization criterion. If this normalization criterion is met for all d_i we can conclude that the aISS flow represents the solution u as a linear combination of eigenfunctions. For more details on the concepts of eigenfunctions we refer to [Ben].

Proposition 4. *If the matrix A is normalized such that*

$$\alpha_i \|Ad_j\|^2 \geq \alpha_j \langle Ad_i, Ad_j \rangle, \tag{4.35}$$

then d_j is an eigenfunction to eigenvalue $\gamma_j = \frac{\alpha_j}{\|Ad_j\|^2}$.

Proof. For d_j to be an eigenfunction to eigenvalue γ_j we need to show that

$$\gamma_j A^T Ad_j \in \partial J(d_j),$$

which by the characterization of the subdifferential means

- If $j > l$:
  - $\langle \gamma_j A^T A d_j, d_j \rangle = \alpha_j$ - which is met for $\gamma_j = \frac{\alpha_j}{\|Ad_j\|^2}$
  - $\langle \gamma_j A^T A d_j, d_i \rangle \leq \alpha_i$ for all i - which substituting the above γ_j is equivalent to

    $$\alpha_i \|Ad_j\|^2 \geq \alpha_j \langle Ad_i, Ad_j \rangle,$$

    and is met by the requirements of the proposition.
- If $j \leq l$:

  $$(\alpha_j - \langle \gamma_j A^T A d_j, d_j \rangle) \leq (\alpha_i - \langle \gamma_j A^T A d_j, d_i \rangle), \ \forall i$$

  For $\gamma_j = \frac{\alpha_j}{\|Ad_j\|^2}$ the left hand side is zero and the condition becomes

  $$\alpha_i \|Ad_j\|^2 \geq \alpha_j \langle Ad_i, Ad_j \rangle,$$

  which again is the propositions requirement.

□

Notice that in the simplest case of ℓ^1 regularization, where d_i are just the (positive and negative) unit normal vectors and $\alpha_i = 1$, the criterion is met if $\|Ae_i\|^2 = 1$, which was discovered in [Ben] before.

5 Scale Space Flows for Polyhedral Functions

In this section we will briefly discuss that the popular scale space flow (also called gradient flow) can also be interpreted under the framework presented above. The scale space flow

$$\partial u(t) = -p(t) \qquad \text{such that } p(t) \in \partial J(u(t)), \tag{5.1}$$

with $u(0) = f$ is commonly used for denoising, and can be seen as the continuous gradient descent with respect to the functional J starting at $u = f$. Due to the fact that

$$p(t) \in \partial J(u(t)) \Leftrightarrow u(t) \in \partial J^*(p(t)) \tag{5.2}$$

as well as Theorem 1, which tells us that the convex conjugate of a polyhedral function again is a polyhedral function, we can interpret (5.1) as the inverse scale space flow with respect to $J^*(p)$ and starting subgradient $u(0) = f \in \partial J^*(p(0))$. Notice that the roles of u and p are inverted in comparison to the previous sections. However, interpreting the scale space flow to $J(u)$ as the inverse scale space flow to $J^*(p)$ allows us to apply all the above convergence theory and draw some very interesting conclusions.

Conclusion 3. *Assume that $J^*(0) < \infty$ and $0 \in \partial J^*(0)$, then the scale space flow (5.1) yields extinction of u in finite time. Furthermore, Theorem 4 gives us the estimate*

$$\|p\|^2 \leq \frac{2D^f_{J^*}(\tilde{p}, p_0)}{t^{k+1}} \tag{5.3}$$

In particular, for regularizations of the form $J(u) = \|Ku\|_1$ (like anisotropic total variation), we have $\tilde{p} = 0$ and $J^*(p) = 0$ for all p in the feasible region, yielding

$$\|p\|^2 \leq 2\frac{J^*(0) - J^*(p_0) - \langle f, 0 - p_0\rangle}{t^{k+1}} = \frac{2J(f)}{t^{k+1}} \tag{5.4}$$

In terms of the computational expenses to determine the scale space flow, it seems that the number of discrete steps the aISS algorithm has to take to reach extinction is much more relevant than the total time, because in between the steps u evolves linearly and p stays constant. The following result shows, that the flow does not take any superfluous steps:

Theorem 6. *Let J^* be an indicator function of some convex bounded polyhedral set, i.e. let the fg-representation of J^* be*

$$J^*(p) = \begin{cases} 0 & \text{if } p = \sum_{i=1}^l \lambda_i d_i,\ \lambda_i \geq 0, \sum_{i=1}^l \lambda_i = 1 \\ \infty & \text{else.} \end{cases} \tag{5.5}$$

Then the index set $I_1(t) = \{1 \leq i \leq l\ :\ \langle u(t), d_i\rangle = \max_j \langle u(t), d_j\rangle\}$ corresponding to the flow (5.1) *is strictly increasing. Thus, the aISS algorithm converges after at most l steps.*

Proof. Let $i \in I_1(t^k)$. We will show that $i \in I_1(t^{k+1})$. Due to $i \in I(t^k)$ we know that $\langle u(t^k), d_i\rangle = r = \langle u(t^k), d_j\rangle$ for all $j \in I_1(t^k)$. Based on the aISS algorithm, $p(t^k)$ is determined as

$$p(t^k) = \arg\min \|DP_{I_1(t^k)}\lambda\|^2 \text{ such that } \lambda_i \geq 0,\ \sum_i \lambda_i = 1. \tag{5.6}$$

Notice that

$$\begin{aligned} \arg\min_\lambda \|DP_{I_1(t^k)}\lambda\|^2 &= \arg\min \|DP_{I_1(t^k)}\lambda\|^2 + \|u(t^k)\|^2 - 2r \\ &= \arg\min_\lambda \|DP_{I_1(t^k)}\lambda\|^2 + \|u(t^k)\|^2 - 2r\sum_j \lambda_j \\ &= \arg\min_\lambda \|DP_{I_1(t^k)}\lambda\|^2 + \|u(t^k)\|^2 - 2\sum_j \lambda_j \langle u(t^k), d_j\rangle \\ &= \arg\min_\lambda \|DP_{I_1(t^k)}\lambda - u(t^k)\|^2 \end{aligned}$$

Therefore, $p(t^k)$ is the projection of $u(t^k)$ onto the convex hull of the d_j, $j \in I(t^k)$, i.e. of the d_j for which $\langle u(t^k), d_j\rangle = r = \max_j \langle u(t^k), d_j\rangle$. Naturally, $\lambda_j > 0$ for all $j \in I(t^k)$. We have seen in the proof of the aISS algorithm above already, that $\lambda_j > 0$ at t^k implies that $j \in I_1(t^{k+1})$. This shows that $I(t)$ is increasing. The fact that $I(t)$ strictly increases at the time steps t^k comes from the definition of t^k (as the next time a new coefficient enters an index set). □

It is very interesting to see that the scale space flow for these kinds of regularizations (where J^* has an fg-representation with $l = m$) not only leads to a monotonically increasing index set, but even allows to conclude the equivalence between the solution to the scale space flow $u(t)$ at time t and the solution to an unconstrained minimization problem as the following theorem tells us.

Theorem 7. *Let the assumptions of Theorem 6 be satisfied. Then the solution $u(t)$ to the scale space flow* (5.1) *satisfies*

$$u(t) = \arg\min_u \frac{1}{2}\|u - f\|^2 + tJ(u) \tag{5.7}$$

Proof. We have seen above that the solution $u(t)$ to (5.1) is piecewise linear in time, more precisely

$$\begin{aligned} u(t) &= u(t^k) - (t - t^k)p(t^k), \\ &= u(0) - (t - t^k)p(t^k) - \sum_{i=1}^{k}(t^i - t^{i-1})p(t^{i-1}). \\ &= f - (t - t^k)p(t^k) - \sum_{i=1}^{k}(t^i - t^{i-1})p(t^{i-1}). \end{aligned}$$

The optimality condition to (5.7) is

$$\frac{1}{t}(u - f) \in -\partial J(u), \tag{5.8}$$

such that it is sufficient to show that $\frac{1}{t}\big((t - t^k)p(t^k) + \sum_{i=1}^{k}(t^i - t^{i-1})p(t^{i-1})\big) \in \partial J(u)$. For the simplicity of being able to also include the first term in the sum, let us (under slight abuse of notation) denote $t^{k+1} = t$ without necessarily meaning the next time step with this notation. Let $p(t^i) = \sum_j \lambda_j^{(i)} d_j$ be the ic-representations with $\lambda_j^{(i)} \geq 0$, $\sum_j \lambda_j^{(i)} = 1$. We can write

$$\begin{aligned} \sum_{i=1}^{k+1} \frac{t^i - t^{i-1}}{t^{k+1}} p(t^{i-1}) &= \sum_{i=1}^{k+1} \frac{(t^i - t^{i-1})}{t^{k+1}} \sum_j \lambda_j^{(i)} d_j \\ &= \sum_j \underbrace{\Big(\sum_{i=1}^{k+1} \frac{(t^i - t^{i-1})}{t^{k+1}} \lambda_j^{(i)}\Big)}_{\tilde{\lambda}_j} d_j \end{aligned} \tag{5.9}$$

We have written the element we would like to show to be in the subdifferential $\partial J(u(t))$ as the sum of the d_j and coefficients $\tilde{\lambda}_j$. We now need to show that $\tilde{\lambda}_j \geq 0$, $\sum_j \tilde{\lambda}_j = 1$ and $\tilde{\lambda}_j = 0$ if $\langle u(t), d_j \rangle < \max_k \langle u(t), d_k \rangle$.

- The first point, $\tilde{\lambda}_j \geq 0$, is obvious because $t^i > t^{i-1}$ and $\lambda_j^{(i)} \geq 0$.

- For the sum to one criteria we have

$$\begin{aligned}
\sum_j \tilde{\lambda}_j &= \sum_j \sum_{i=1}^{k+1} \frac{(t^i - t^{i-1})}{t^{k+1}} \lambda_j^{(i)} \\
&= \sum_{i=1}^{k+1} \frac{(t^i - t^{i-1})}{t^{k+1}} \underbrace{\sum_j \lambda_j^{(i)}}_{=1} \\
&= \frac{1}{t^{k+1}} \sum_{i=1}^{k+1} (t^i - t^{i-1}) \\
&= 1 \qquad (5.10)
\end{aligned}$$

- Finally, we have to show that at indices j at which $\langle u(t), d_j \rangle < \max_k \langle u(t), d_k \rangle$, we have $\tilde{\lambda}_j = 0$, or in other words $\tilde{\lambda}_j = 0$ for $j \notin I_1(t)$. Now, Theorem 6 tells us that $I_1(t)$ is strictly increasing. Therefore, if $j \notin I_1(t)$ we can conclude $j \notin I_1(t^i)$ for all $t^i \leq t$, which means $\lambda_j^{(i)} = 0$ for all i. Thus $\tilde{\lambda}_j = \sum_{i=1}^{k+1} \frac{(t^i - t^{i-1})}{t^{k+1}} \lambda_j^{(i)} = 0$ if $j \notin I_1(t)$, which concludes our proof.

□

Finally, let us mention that many regularizations meet the assumptions of Theorem 6 that J^* is an indicator function of some convex bounded polyhedral set. Consider for instance $J(u) = \|Tu\|_1$ for any matrix T (for instance with T being the discrete approximation of the gradient and thus $J(u)$ being anisotropic total variation regularization). For such a J the convex conjugate is

$$\begin{aligned}
J^*(p) &= \sup_u \left(\langle p, u \rangle - \|Tu\|_1 \right) \\
&= \sup_u \inf_{\|q\|_\infty \leq 1} \langle p - T^T q, u \rangle
\end{aligned}$$

Thus, we have $J^*(p) = 0$ if and only if $p \in \{T^T q \mid \|q\|_\infty \leq 1\}$ (which clearly is a bounded polyhedral set) and $J^*(p) = \infty$ else. A similar argument shows that the assumptions of Theorem 6 are also met for $J(u) = \|Tu\|_\infty$.

For T being the discrete approximation of the divergence, we have confirmed and generalized the result from [BCNO] in which the authors have shown the equivalence of the scale space flow and the minimizer of the energy for the particular case of $J(u) = \|\text{div}(u)\|_1$.

6 Examples and Numerical results

6.1 A first example in 2d

Let us give an example of a more complicated polyhedral function than the ℓ^1 norm, particularly to illustrate the use of the $\sum_{i=1}^{l} \lambda_i = 1$ constraint.

Example 4. Let us consider the following convex polyhedral function in two dimensions given in its fg-representation by $l = 6$, $\alpha_1 = 1$, $\alpha_2 = 1$, $\alpha_3 = 2$,

$\alpha_4 = 1$, $\alpha_5 = 1$, $\alpha_6 = 0$, $\alpha_7 = \infty$, $\alpha_8 = \infty$, $\alpha_9 = \infty$, $\alpha_{10} = \infty$, $\alpha_{11} = 2$, and

$$d_1 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, d_2 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, d_3 = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$
$$d_4 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, d_5 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, d_6 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$d_7 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, d_8 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, d_9 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, d_{10} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
$$d_{11} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Figure 1 illustrates the area where $J(u) < \infty$ as well as the d_i.

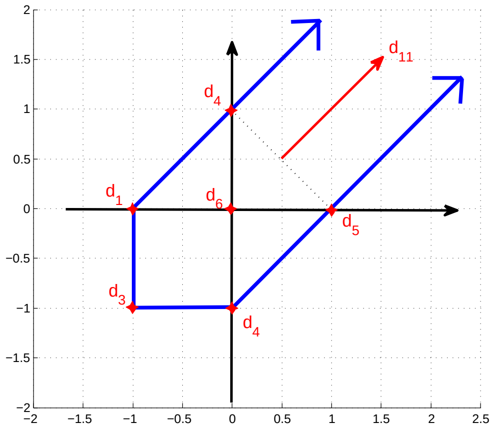


Figure 1: Illustrating the fg-representation of $J(u)$

Let us look at two numerical experiments we can do with the polyhedral function above:

1. Projection onto the feasible region

First let us choose A to be the identity and $f = (1, -1.5)^T$ to lie outside of the $J(u) < \infty$ region. As we have seen above, the aISS flow will converge to a $u \in \arg\min_{J(u)<\infty} \|f - u\|^2$, which has a unique solution, namely the projection of f onto the $J(u) < \infty$ region. As we can see in Figure 2 the algorithm converges in two steps. First it chooses the edge d_2 since the product $\langle d_2, f\rangle$ is largest. Next it includes $i = 4$ in the index set of possibly non-zero elements and finds the projection of f to be in the convex hull of d_2 and d_4, thus having fully converged.

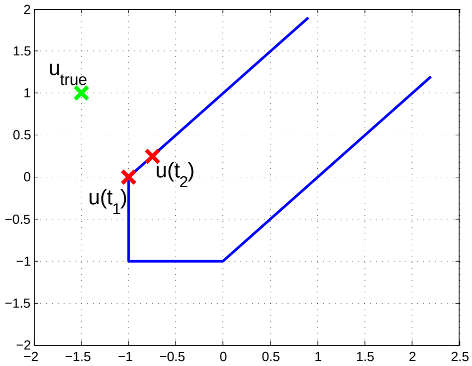


Figure 2: Iterates of the aISS algorithm for the calculation of a projection

2. Finding the J-minimizing solution

In the second experiment, we choose A as a random 2×2 matrix with values drawn from a standard Gaussian distribution and generate the data f as $f = Au_{\text{true}}$ for $u_{\text{true}} = (1, 1)^T$. Since now the true solution lies in the feasible region, we expect the aISS algorithm to converge to u_{true}, which is indeed the case, as we can see in Figure 3. This time aISS took three steps. First, d_4 enters the index set I_1 and simultaneously makes $d_6 = 0$ leave I_2. Next the coefficient corresponding to d_{11} is allowed to be non-zero. Although $u_{\text{true}} = d_{11}$, the algorithm can not yet fully converge because $I_1 = \{4\}$ and due to the sum to one constraint for indices in I_1 the solution $u(t_2)$ at the second time step is of the form $d_4 + \lambda_{11} d_{11}$. Finally, at the third time step $i = 6$ reenters the index set I_2 and allows $u(t_3) = d_{11} = u_{\text{true}}$.

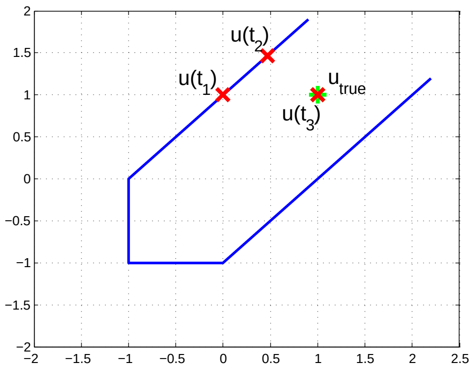


Figure 3: Iterates of the aISS algorithm for the calculation a J-minimizer of $Au = f$

6.2 Convex hull constraints

While the previous example was instructive, it only served illustration purposes, since a minimization over a vector of length 2 is of little practical relevance due to its low dimensionality. Frequently arising in optimization are quadratic programming problems of the form

$$\min_u \|Au - f\|^2 \qquad \text{such that } u \in C, \tag{6.1}$$

where C is some given polyhedron. Generally, there are two different ways to express polyhedra, either by inequalities (a so called H-representation $C = \{u \mid B_1 u \leq b_1,\ B_2 u = b_2\}$) or as a convex hull (a so called V-representation $C = \{u \mid u = D\lambda,\ \lambda_i \geq 0,\ \sum_i \lambda_1 = 1\}$). For the inverse scale space flow a V-representation is very well suited because it immediately gives a fg-representation of the regularizing function. Notice that the conversion of one polyhedral representation into the other can be extremely computationally challenging such that one should keep the polyhedron in the format that naturally arises in the application and solve the corresponding problem (6.1). Many methods deal with incorporating polyhedral constraints in H-representation such that aISS offers a fast algorithm for C given in V-representation. The inverse scale space flow will particularly be fast, if the true solution lies on a low dimensional face of C, i.e. if $u = D\lambda$ with only few non-zero λ_i.

For quadratic programming problems in H-representation Matlab offers an optimization method called *quadprog*. In the following we would like to compare the inverse scale space flow for solving a constrained optimization problem with the Matlab algorithm. Due to the different representations the two algorithms expect, we need to choose an example problem for which both representations are easily computable. Let us consider

$$\min_u \|Au - f\|^2 \qquad \text{such that } u \geq 0,\ \sum_i u_i = 1. \tag{6.2}$$

The constraints can either be represented by $C = \{u \mid B_1 u \leq b_1,\ B_2 u = b_2\}$ with $B_1 = -I$ being the negative identity, $b_1 = 0$, $B_2 = \mathbb{1}$ being a row vector with all ones and $b_2 = 1$, or as $C = \{u \mid u = D\lambda,\ \lambda_i \geq 0,\ \sum_i \lambda_1 = 1\}$ with $D = I$ being the identity. Notice that this is special case where the number of vertices in the V-representation (number of columns in D) and number of intersecting hyperplanes in the H-representation (number of rows of B_1 and B_2) is almost the same and both representations are easily computable.

For our numerical experiment we choose A to be a random $n \times m$ matrix and random data f, both with values from a uniform sampling of $[0, 1]$. Table 6.2 shows a run time comparison of the two methods for different matrix sizes, where we ran each experiment 10 times and took the average values for the run time (in seconds) and sparsity.

Matrix size	100×200	180×200	100×250	50×200	100×300
Runtime aISS	0.33	0.28	0.27	0.17	0.30
Runtime quadprog	4.0	2.3	7.1	3.2	17.5
$\|u\|_0$	18.8	27.6	21.5	16	22.2

We can see that the aISS flow determined the solution to the constrained optimization problem much faster than the Matlab algorithm. Moreover, due to the sparsity of the solution remaining rather low even for increasing dimensions, the run time of the aISS algorithm is almost not affected by the changes in matrix dimension, while *quadprog* has difficulties dealing with the large underdetermined 100×300 system. For *quadprog* to converge we even had to increase the maximum number of iteration. A further increase in dimensionality is basically impossible with *quadprog*, while it is no problem for aISS.

6.3 Linear inequality constraints

As we have seen in the previous subsection, the aISS algorithm can handle convex hull constraints very well, since it immediately gives us a fg-representation of the polyhedral regularizer. We will see in this subsection, that the problem

$$\min_u \|Au - f\|^2 \qquad \text{such that } Bu \leq b \tag{6.3}$$

for an injective A is also easy to handle for the aISS algorithm, by going to the dual formulation. Let us define

$$\begin{aligned} H(u) &= \frac{1}{2}\|Au - f\|^2 \\ J(Bu) &= \begin{cases} 0 & \text{if } Bu \leq b \\ \infty & \text{else} \end{cases} \end{aligned} \tag{6.4}$$

Fenchels duality theorem (cf. [ET99])allows us to conclude that

$$\min_u H(u) + J(Bu) = -\min_q H^*(-T^T q) + J^*(q), \tag{6.5}$$

where the superscript * denotes the convex conjugate functionals. We have

$$H^*(p) = \sup_u \{\langle p, u\rangle - H(u)\} \tag{6.6}$$

The supremum yields the optimality condition, which for injective A can be solved for the optimal u:

$$\begin{aligned} & 0 = p - A^T(Au - f) \\ \Rightarrow \quad & u = (A^T A)^{-1}(A^T f + p) \end{aligned} \tag{6.7}$$

Inserting back into H^* we can calculate

$$\begin{aligned} H^*(p) &= \langle p, (A^T A)^{-1}(A^T f + p)\rangle - \frac{1}{2}\|A(A^T A)^{-1}(A^T f + p) - f\|^2 \\ &= \frac{1}{2}\|A(A^T A)^{-1} p + (2I - A(A^T A)^{-1} A^T) f\|^2 + C, \end{aligned} \tag{6.8}$$

where C is some constant independent of p. Another calculation shows that

$$J^*(p) = \begin{cases} \langle b, p\rangle & \text{if } p_i \geq 0 \\ \infty & \text{else} \end{cases}. \tag{6.9}$$

Therefore, we can conclude

Proposition 5. *For an injective matrix A the problems*

$$\tilde{u} = \arg\min_u \|Au - f\|^2 \qquad \textit{such that } Bu \leq b \tag{6.10}$$

and

$$\tilde{q} = \arg\min_q \left\{ \begin{array}{c} \frac{1}{2}\|A(A^T A)^{-1} B^T q - (2I - A(A^T A)^{-1} A^T) f\|^2 + \langle b, q\rangle \\ \textit{such that } q_i \geq 0 \end{array} \right\} \tag{6.11}$$

are equivalent with the relation

$$\tilde{u} = (A^T A)^{-1}(A^T f - B^T \tilde{q}) \tag{6.12}$$

between the primal and dual variable.

The above proposition allows us to rewrite inequality constraints into a problem of the form (6.11), which can easily be solved by the adaptive inverse scale space method, since it is nothing but a non-negative least squares problem.

Matlab provides two function, *quadprog* and *lsqlin*, to solve the constrained problem (6.10). For a numerical test we chose a Matrix $A \in \mathbb{R}^{n \times m}$ with values drawn from a Gaussian normal distribution, where $n \geq m$ to guarantee injectivity. We generated the data $f = Au$ with a vector $u \in \mathbb{R}^m$ coming from a normal distribution. Similarly, the inequality constraints were chosen from random $B \in R^{k \times m}$, $b \in R^k$, again from a normal distribution. We used $k < m$ to guarantee that the set $\{u \mid Bu \leq b\}$ is non-empty. Table 6.3 shows the run times in seconds for different values of (n, m, k).

(n,m,k)	**(400,200,100)**	**(300,290,200)**	**(400,400,100)**	**(400,110,100)**
aISS	0.26	1.49	0.36	0.26
quadprog	1.25	4.92	5.56	0.60
lsqlin	2.11	6.25	7.18	0.97

We can see that aISS outperformed the Matlab algorithms in all test cases. Particularly in the case of a big quadratic A aISS was much faster needing less than 1/10 of the time that *quadprog* needed. Generally, we should metion, that aISS is particularly fast, if q in the formulation (6.11) is sparse. Since q can also be interpreted as the Lagrange multiplier to enforce $Bu \leq b$, this means that aISS is particularly fast, if the constraint has to be enforced only at few indices.

6.4 Some examples in applications

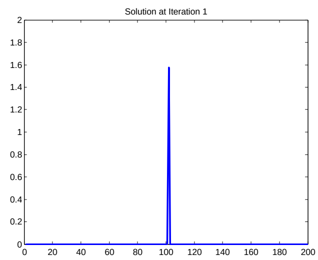
In this final section of our numerical results we provide some examples of polyhedral regularized functions for problems that could come up in applications.

6.4.1 Non-negative ℓ^1 minimization

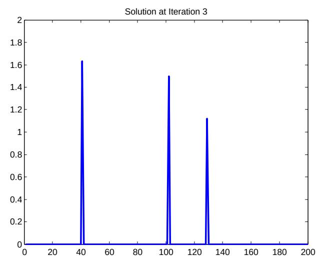
The example of using aISS for unconstrained ℓ^1 minimization has extensively been studied in [BMBO11]. It is easy to see that an additional non-negativity constraint is straight forward to include. While the fg-representation of the ℓ^1 norm contains all positive and negative Euclidean normal vectors, e_i and $-e_i$, we can simply omit the negative ones to obtain the fg-representation of

$$J(u) = \begin{cases} \|u\|_1 & \text{if } u \geq 0, \\ \infty & \text{else.} \end{cases} \tag{6.13}$$

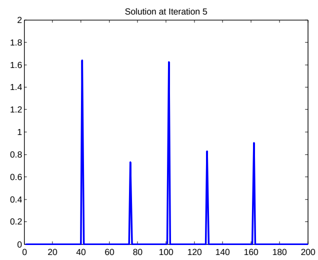
As a simple example, we generated a random $A \in R^{100 \times 200}$ with values from a Gaussian distribution, and data $f = Au_{true}$ with u_{true} consisting of 8 positive entries from a uniform sampling of $[0, 2]$ at random indices. Figure, 4 shows the results of the aISS algorithm after 1, 3, 5 and 8 iterations.



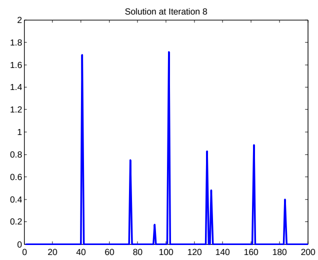
(a) Iteration 1



(b) Iteration 3



(c) Iteration 5



(d) Iteration 8

Figure 4: Intermediate results for determining non-negative ℓ^1 minimizing solutions

We can see that similar to the aISS results from [BMBO11], we reconstruct one peak at each iteration. For sparse solutions like in this example, aISS is extremely fast, since it works on very low dimensions based on the indices where the subgradient is one.

6.4.2 Projection onto the ℓ^1 ball and ℓ^∞ minimization

We have shown in [BMBO11] that the aISS framework not only works for determining ℓ^1 minimizing solutions, but also for unconstrained problems of the form $\min_u \|Au - f\|^2 + \mu\|u\|_1$. Similarly, one could consider the regularizing constraint $\min_u \|Au - f\|^2$ such that $\|u\|_1 \leq 1$ (or less than a parameter μ which could however also be incorporated by rescaling A). Notice that the fg-representation of the ℓ^1 ball is easy to determine since it consists of all positive and negative unit normal vectors and (additionally) the vector with 0 in all components, together with $l = m$ and $\alpha_i = 0$ for all i, which makes it well suited for the aISS algorithm.

Furthermore, notice that the dual formulation for the problem

$$\min_{\|p\|_1 \leq 1} \|\alpha T^T p - f\|^2, \tag{6.14}$$

is an ℓ^∞ regularized problem with the matrix T, i.e.

$$\min_u \|u - f\|^2 + \alpha\|Tu\|_\infty. \tag{6.15}$$

Respectively, unconstrained ℓ^1 minimization by duality is equivalent to the constrained ℓ^∞ formulation

$$\min_u \|u - f\|^2 \qquad \text{such that } \|Tu\|_\infty \leq \mu, \tag{6.16}$$

such that the aISS method is also very useful for possible regularizations involving the ℓ^∞ norm. As a toy example let us consider the problem of denoising smooth signals by penalizing with the ℓ^∞ norm of the second derivative, i.e. minimizing (6.15) with T being the discretization of the (one dimensional) Laplacian. Figure 5 gives an example of such a denoising result for a sine function.

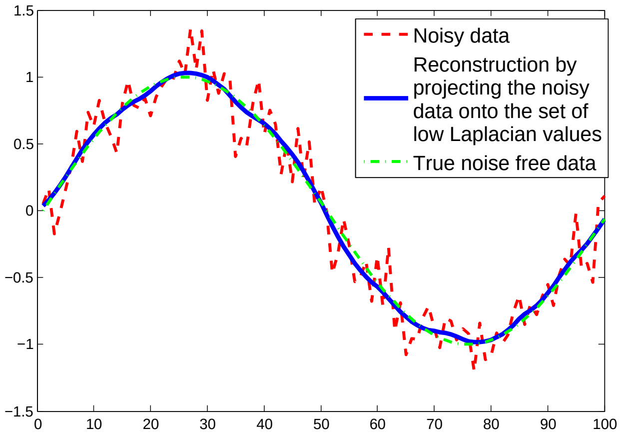


Figure 5: Denoising a function by restricting the maximum Laplacian

6.4.3 Best convex approximation

Knowing the characterization of convex functions as functions for which the second derivative is non-negative, we could also use the discretization of the second derivative operator T from the previous example to find the best convex approximation of a function by minimizing

$$\min_u \|u - f\|^2 \qquad \text{such that } Tu \geq 0. \tag{6.17}$$

Notice that (6.17) has the form of the problems investigated in Section 6.3 and again can rapidly be solved with aISS. Figure 6 shows an example of denoising the function $f(x) = x^2$ with (6.17), i.e. by using the prior knowledge that the true function we are looking for is convex.

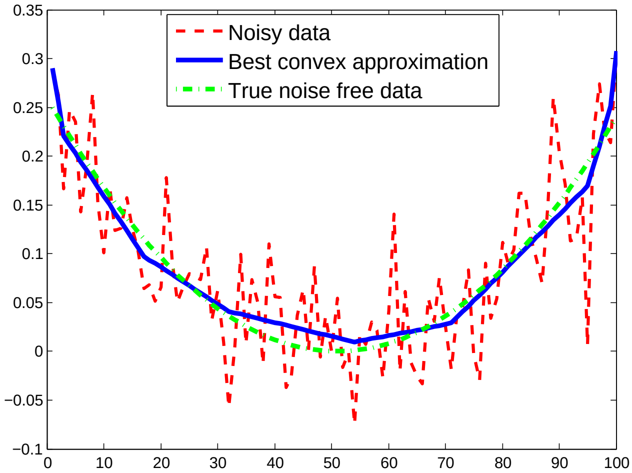


Figure 6: Determining the best convex approximation

6.4.4 Best monotone approximation

Similar to the previous example, one could also look for the best monotone approximation by replacing the discrete Laplace operator from the previous subsection with the discrete derivative and again solve the resulting system with aISS. Figure 7 shows an example of such a monotone approximation result. The minimizer will typically have staircases - in case a smooth underlying function can be expected, one would have to add an additional smoothness term for instance by combining this approach with the one from Section 6.4.2.

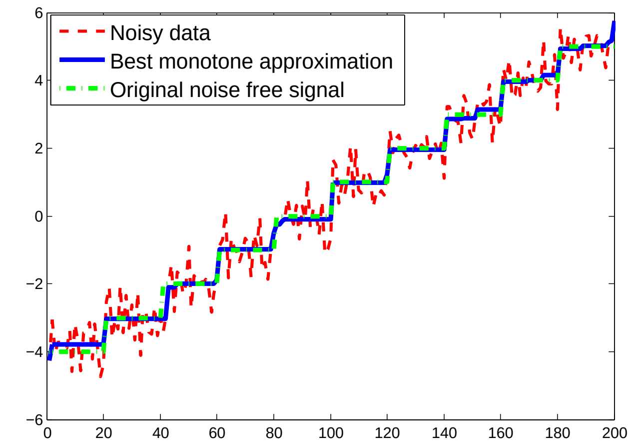


Figure 7: Determining the best monotone approximation

7 Conclusions

We have generalized the concept of solving the inverse scale space flow exactly from ℓ^1 regularization to arbitrary polyhedral functions. Although the inverse scale space flow at first seems to be difficult to solve due to the differential inclusion, we have seen that it can easily be solved exactly for any convex polyhedral function in fg-representation. We proved finite time convergence and presented a general adaptive inverse scale space algorithm only depending on the fg-representation of the polyhedral function. The connection to the forward scale space flow was made by showing that it corresponds to the inverse scale space flow on the convex conjugate problem. Numerical examples show that the aISS can efficiently compute a wide variety of different regularized or constrained problems, if the fg-representation is accessible and the solution is sparse in the ic-representation.

In future research we will investigate if the inverse scale space flow might also allow fast and exact solutions for non-quadratic fidelity terms.

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