1	Superiorization: An optimization heuristic for medical physics
2	Gabor T. Herman <sup>*</sup>
3	Department of Computer Science, The Graduate Center,
4	City University of New York, New York, NY 10016, USA
5	Edgar Garduño
6	Departamento de Ciencias de la Computación,
7	Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas,
8	Universidad Nacional Autónoma de México,
9	Cd. Universitaria, C.P. 04510, Mexico City, Mexico
10	Ran Davidi
11	Department of Radiation Oncology, Stanford University, Stanford, CA 94305, USA
12	Yair Censor
13	Department of Mathematics, University of Haifa, Mt. Carmel, 31905 Haifa, Israel
14	$\mathbf{Purpose}$ : To describe and mathematically validate the superiorization methodol-
15	ogy, which is a recently-developed heuristic approach to optimization, and to discuss
16	its applicability to medical physics problem formulations that specify the desired
17	solution (of physically given or otherwise obtained constraints) by an optimization
18	criterion.
19	Methods: The superiorization methodology is presented as a heuristic solver for
20	a large class of constrained optimization problems. The constraints come from the
21	desire to produce a solution that is constraints-compatible, in the sense of meeting
22	requirements provided by physically or otherwise obtained constraints. The underly-
23	ing idea is that many iterative algorithms for finding such a solution are perturbation
24	resilient in the sense that, even if certain kinds of changes are made at the end of
25	each iterative step, the algorithm still produces a constraints-compatible solution.
26	This property is exploited by using permitted changes to steer the algorithm to a
27	solution that is not only constraints-compatible, but is also desirable according to
28	a specified optimization criterion. The approach is very general, it is applicable to

29 many iterative procedures and optimization criteria used in medical physics.

30 **Results**: The main practical contribution is a procedure for automatically pro-31 ducing from any given iterative algorithm its superiorized version, which will supply 32 solutions that are superior according to a given optimization criterion. It is shown 33 that if the original iterative algorithm satisfies certain mathematical conditions, then 34 the output of its superiorized version is guaranteed to be as constraints-compatible as the output of the original algorithm, but it is superior to the latter according to the 35 36 optimization criterion. This intuitive description is made precise in the paper and 37 the stated claims are rigorously proved. Superiorization is illustrated on simulated 38 computerized tomography data of a head cross-section and, in spite of its general-39 ity, superiorization is shown to be competitive to an optimization algorithm that is 40 specifically designed to minimize total variation.

41 Conclusions: The range of applicability of superiorization to constrained opti42 mization problems is very large. Its major utility is in the automatic nature of
43 producing a superiorization algorithm from an algorithm aimed at only constraints44 compatibility; while non-heuristic (exact) approaches need to be redesigned for a new
45 optimization criterion. Thus superiorization provides a quick route to algorithms for
46 the practical solution of constrained optimization problems.

47 Keywords: superiorization, constrained optimization, heuristic optimization, tomography,48 total variation

49

## I. INTRODUCTION

50 Optimization is a tool that is used in many areas of Medical Physics. Prime examples are 51 radiation therapy treatment planning and tomographic reconstruction, but there are others 52 such as image registration. Some well-cited classical publications on the topic are<sup>1-12</sup> and 53 some recent articles are<sup>13-26</sup>.

54 In a typical medical physics application, one uses *constrained optimization*, where the 55 constraints come from the desire to produce a solution that is *constraints-compatible*, in 56 the sense of meeting the requirements provided by physically or otherwise obtained con-57 straints. In radiation therapy treatment planning, the requirements are usually in the form

58 of constraints prescribed by the treatment planner on the doses to be delivered at specific 59 locations in the body. These doses in turn depend on information provided by an imaging instrument, typically a Magnetic Resonance Imaging (MRI) or a Computerized Tomogra-60 phy (CT) scanner. In tomography, the constraints come from the detector readings of the 61 instrument. In such applications, it is typically the case that a large number of solutions 62 would be considered good enough from the point of view of being constraints-compatible; 63 to a large extent, but not entirely, due to the fact that there is uncertainty as to the exact 64 65 nature of the constraints (for example, due to noise in the data collection). In such a case, an optimization criterion is introduced that helps us to distinguish the "better" constraints-66 compatible solutions (for example, this criterion could be the total dose to be delivered to 67 the body, which may vary quite a bit between radiation therapy treatment plans that are 68 compatible with the constraints on the doses delivered to individual locations). 69

The superiorization methodology (see, for example,<sup>22,27–32</sup>) is a recently-developed heuristic approach to optimization. The word *heuristic* is used here in the sense that the process is not guaranteed to lead to an optimum according to the given criterion; approaches aimed at processes that are guaranteed in that sense are usually referred to as *exact*. Heuristic approaches have been found useful in practical applications of optimization, mainly because they are often computationally much less expensive than their exact counterparts, but nevertheless provide solutions that are appropriate for the application at hand<sup>33–35</sup>.

77 The underlying idea of the superiorization approach is the following. In many applications there exists a computationally-efficient iterative algorithm that produces a constraints-78 79 compatible solution for the given constraints. (An example of this for radiation therapy treatment planning is reported in<sup>36</sup>, its clinical use is discussed in<sup>15</sup>.) Furthermore, often 80 81 the algorithm is *perturbation resilient* in the sense that, even if certain kinds of changes are made at the end of each iterative step, the algorithm still produces a constraints-compatible 82 solution<sup>27–30</sup>. This property is exploited in the superiorization approach by using such per-83 84 turbations to steer the algorithm to a solution that is not only constraints-compatible, but is also desirable according to a specified optimization criterion. The approach is very general, 85 86 it is applicable to many iterative procedures and optimization criteria.

87 The current paper presents a major advance in the practice and theory of superiorization.
88 The previous publications<sup>22,27–32</sup> used the intuitive idea to present some superiorization
89 algorithms, in this paper the reader will find a totally automatic procedure that turns an

iterative algorithm into its superiorized version. This version will produce an output that 90 is as constraints-compatible as the output of the original algorithm, but it is superior to 91 92 that according to an optimization criterion. This claim is mathematically shown to be 93 true for a very large class of iterative algorithms and for optimization criteria in general, typical restrictions (such as convexity) on the optimization criterion are not essential for 94 the material presented below. In order to make precise and validate this broad claim, we 95 present here a new theoretical framework. The framework  $of^{29}$  is a precursor of what we 96 97 present here, but it is a restricted one, since it assumes that the constraints can be all satisfied simultaneously, which is often false in medical physics applications. There is no 98 such restriction in the presentation below. 99

100 The idea of designing algorithms that use interlacing steps of two different kinds (in our 101 case, one kind of steps aim at constraints-compatibility and the other kind of steps aim at improvement of the optimization criterion) is well-established and, in fact, is made use of 102 in many approaches that have been proposed with exact constrained optimization in mind; 103 see, for example, the works of Helou Neto and De Pierro<sup>37,38</sup>, of Nurminski<sup>39</sup>, of Combettes 104 and coworkers<sup>40,41</sup>, of Sidky and Pan and coworkers<sup>23,42,43</sup> and of Defrise and coworkers<sup>44</sup>. 105 106 However, none of these approaches can do what can be done by the superiorization approach as presented below, namely the automatic production of a heuristic constrained optimization 107 algorithm from an iterative algorithm for constraints-compatibility. For example, in<sup>37</sup> it is 108 assumed (just as in the theory presented in  $our^{29}$ ) that all the constraints can be satisfied 109 110 simultaneously.

111 A major motivator for the additional theory presented in the current paper is to get rid of this assumption, which is not reasonable when handling real problems of medical physics. 112 Motivated by similar considerations, Helou Neto and De Pierro<sup>38</sup> present an alternative 113 114 approach that does not require this unreasonable assumption. However, in order to solve 115 such a problem, they end up with iterative algorithms of a particular form rather than having 116 the generality of being able to turn any constraints-compatibility seeking algorithm into a superiorized one capable of handling constrained optimization. Also, the assumptions they 117 have to make in order to prove their convergence result (their Theorem 15) indicate that 118 119 their approach is applicable to a smaller class of constrained optimization problems than 120 the superiorization approach whose applicability seems to be more general. However, for the mathematical purist, we point out that they present an exact constrained optimization 121

algorithm, while superiorization is a heuristic approach. Whether this is relevant to medical
physics practice is not clear: exact algorithms are not run forever, but are stopped according
to some stopping-rule, the relevant questions in comparing two algorithms are the quality
of the actual output and the computation time needed to obtain it.

126 Ultimately, the quality of the outputs should be evaluated by some figures of merit relevant to the medical task at hand. An example of a careful study of this kind that 127 involves superiorization is  $in^{30}$  (Section 4.3), which reports on comparing in CT the efficacy 128 129 of constrained optimization reconstruction algorithms for the detection of low-contrast brain tumors by using the method of statistical hypothesis testing (which provides a P-value that 130 indicates the significance by which we can reject the null hypothesis that the two algorithms 131 are equally efficacious in favor of the alternative that one is preferable). Such studies bundle 132 together two things: (i) the formulation of the constrained optimization task and (ii) the 133 performance of the algorithm in performing that task. The first of these requires a translation 134 of the medical aim into a mathematical model, it is important that this model should be 135 appropriately chosen. 136

137 The superiorization approach is not about choosing this model, it kicks in once the model is chosen and aims at producing an output that is "good" according to the mathematical 138 139 specifications of the constraints and of the optimization criterion. Thus superiorization has been used to compare the effects on the quality of the output in CT when the optimization 140 criterion is specified by total variation (TV) versus by entropy<sup>28</sup> or versus by the  $\ell_1$ -norm 141 of the Haar transform<sup>32</sup>. However, the current paper is not about discussing how to trans-142 143 late the underlying medical physics task into a constrained optimization problem. For our purposes here, we are assuming that the mathematical model has been worked out and 144 145 concentrate on the algorithmic approach for solving the resulting constrained optimization 146 problem. We claim that the evaluation of such algorithms should not be based on the 147 medical figures of merit mentioned at the beginning of the previous paragraph, but rather 148 on their performance in solving the mathematical problem. If "good" solutions to the con-149 strained optimization problem are not medically efficacious, that indicates that something is wrong with the mathematical model and not that something is wrong with the algorithmic 150 approach. For this reason, in this paper we will not carry out a careful investigation of the 151 medical efficacy of any algorithm in the manner that we have done in<sup>30</sup> (Section 4.3), but will 152 restrict ourselves to a simple illustration of the performance of the superiorization approach 153

154 as compared to the previously published algorithm of<sup>42</sup> that is aimed at performing exact155 minimization.

Examples of such studies already exist. Superiorization was compared in<sup>27</sup> with Algorithm 156  $6 \text{ of}^{40}$  and  $\text{in}^{45}$  with the algorithm of Goldstein and Osher that they refer to as TwIST<sup>46</sup> with 157 split Bregman<sup>47</sup> as the substep. In both cases the implementation was done by the proposers 158 of the algorithms. In these reported instances superiorization did well: the constraints-159 160 compatibility and the value of the function to be minimized were very similar for the outputs 161 produced by the algorithms being compared, but the superiorization algorithm produced its output four times faster than the alternative. It would be unjustified to draw any general 162 conclusions on the mathematical performance and speed of superiorization based on just a 163 few experiments, but the reported results are encouraging. 164

165 However, the main reason why we advocate superiorization is different from what is 166 discussed above. The reason why we claim it to be helpful in medical physics research is that it has the potential of saving a lot of time and effort for the researcher. Let us consider 167 168 a historical example. Likelihood optimization using the iterative process of expectation maximization (EM)<sup>48</sup> gained immediate and wide acceptance in the emission tomography 169 170 community. It was observed that irregular high amplitude patterns occurred in the image 171 with a large number of iterations, but it was not until five years later that this problem was corrected<sup>49</sup> by the use of a maximum a posteriority probability (MAP) algorithm with 172 173 a multivariate Gaussian prior. Had we had at our disposal the superiorization approach, 174 then the introduction of an optimization criterion (Gaussian or other) into the iterative 175 expectation maximization (EM) process would have been a simple matter and we would have saved the time and effort spent on designing a special purpose algorithm for the MAP 176 formulation. A TV-superiorization of the EM algorithm is presented in<sup>50</sup>. 177

Even though our major claim for superiorization is that it provides a quick route to algorithms for the practical solution of constrained optimization problems, before leaving this introduction let us bring up a question that has to do with the performance of the resulting algorithms: Will superiorization produce superior results to those produced by contemporary MAP methods or is it faster than the better of such methods? At this stage we have not yet developed the mathematical notation to discuss this question in a rigorous manner, we return to it in Subsection II F.

185 In the next section we present in detail the superiorization methodology. In the subse-

186 quent section we provide an illustrative example by reporting on reconstructions produced187 by algorithms applied to simulated computerized tomography data of a head cross-section.188 In the final section we discuss our results and present our conclusions.

189

# II. THE SUPERIORIZATION METHODOLOGY

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#### A. Problem sets, proximity functions and $\varepsilon$ -compatibility

191 Although optimization is often studied in a more general context (such as in Hilbert or 192 Banach spaces), in medical physics we usually deal with a special case, where optimization 193 is performed in a *Euclidean space*  $\mathbb{R}^J$  (the space of *J*-dimensional vectors of real numbers, 194 where *J* is a positive integer). As often appropriate in practice, we further restrict the 195 domain of optimization to a nonempty subset  $\Omega$  of  $\mathbb{R}^J$  (such as the *nonnegative orthant*  $\mathbb{R}^J_+$ 196 that consists of vectors all of whose components are nonnegative).

197 We now turn to formalizing the notion of being compatible with given constraints, a notion that we have used informally in the previous section. In any application, there is a 198 problem set  $\mathbb{T}$ ; each problem  $T \in \mathbb{T}$  is essentially a description of the constraints in that 199 particular case. For example, for a tomographic scanner, the problem of reconstruction for 200 a particular patient at a particular time is determined by the measurements taken by the 201 scanner for that patient at that time. The intuitive notion of constraints-compatibility is 202 formalized by the use of a proximity function  $\mathcal{P}r$  on  $\mathbb{T}$  such that, for every  $T \in \mathbb{T}$ ,  $\mathcal{P}r_T$ 203 maps  $\Omega$  into  $\mathbb{R}_+$ , the set of nonnegative real numbers; i.e.,  $\mathcal{P}r_T: \Omega \to \mathbb{R}_+$ . Intuitively we 204 205 think of  $\mathcal{P}r_T(\boldsymbol{x})$  as an indicator of how incompatible  $\boldsymbol{x}$  is with the constraints of T. For example, in tomography,  $\mathcal{P}r_T(\boldsymbol{x})$  should indicate by how much a proposed reconstruction 206 207 that is described by an  $\boldsymbol{x}$  in  $\Omega$  violates the constraints of the problem T that are provided 208 by the measurements taken by the scanner. For example, if we use b to denote the vector of estimated line integrals based on the measurements obtained by the scanner and by A209 210 the system matrix of the scanner, then a possible choice for the proximity function is the norm-distance  $\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|$ , which we will use as an example in the discussions that follow. 211 212 An alternative legitimate choice for the proximity function is the Kullback-Leibler distance  $KL(\boldsymbol{b}, \boldsymbol{Ax})$ , which is the negative log-likelihood of a statistical model in tomography. The 213 special case  $\mathcal{P}r_{T}(\boldsymbol{x}) = 0$  is interpreted by saying that  $\boldsymbol{x}$  is perfectly compatible with the 214

215 constraints; due to the presence of noise in practical applications, it is quite conceivable 216 that there is no  $\boldsymbol{x}$  that is perfectly compatible with the constraints, and we accept an  $\boldsymbol{x}$ 217 as constraints-compatible as long as the value of  $\mathcal{P}r_T(\boldsymbol{x})$  is considered to be small enough 218 to justify that decision. Combining these two concepts leads to the notion of a *problem* 219 *structure*, which is a pair  $\langle \mathbb{T}, \mathcal{P}r \rangle$ , where  $\mathbb{T}$  is a nonempty problem set and  $\mathcal{P}r$  is a proximity 210 function on  $\mathbb{T}$ . For a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$ , a problem  $T \in \mathbb{T}$ , a nonnegative  $\varepsilon$  and an 221  $\boldsymbol{x} \in \Omega$ , we say that  $\boldsymbol{x}$  is  $\varepsilon$ -compatible with T provided that  $\mathcal{P}r_T(\boldsymbol{x}) \leq \varepsilon$ .

As an example (whose applicability to tomographic reconstruction is illustrated in Section 223 III), consider the problem structure that arises from the desire to find nonnegative solutions 224 of sequences of blocks of linear equations. Then the appropriate choices are  $\Omega = \mathbb{R}^J_+$  and 225 the problem structure is  $\langle \mathbb{S}, Res \rangle$ , where the problem set  $\mathbb{S}$  is

$$S = \left\{ \left( \left\{ \left( \boldsymbol{a}^{1}, b_{1} \right), \dots, \left( \boldsymbol{a}^{\ell_{1}}, b_{\ell_{1}} \right) \right\}, \dots, \left\{ \left( \boldsymbol{a}^{\ell_{1} + \dots + \ell_{W-1} + 1}, b_{\ell_{1} + \dots + \ell_{W-1} + 1} \right), \dots, \left( \boldsymbol{a}^{\ell_{1} + \dots + \ell_{W}}, b_{\ell_{1} + \dots + \ell_{W}} \right) \right\} \right) \right|$$

$$W \text{ is a positive integer and,} \qquad (1)$$
for  $1 \leq w \leq W$ ,  $\ell_{w}$  is a positive integer and,  
for  $1 \leq i \leq \ell_{1} + \dots + \ell_{W}$ ,  $\boldsymbol{a}^{i} \in \mathbb{R}^{J}$  and  $b_{i} \in \mathbb{R} \right\}$ 

**226** and the proximity function Res on  $\mathbb{S}$  is defined, for any problem  $S = (\{(\boldsymbol{a}^1, b_1), \dots, (\boldsymbol{a}^{\ell_1}, b_{\ell_1})\}, \dots, \{(\boldsymbol{a}^{\ell_1 + \dots + \ell_{W-1} + 1}, b_{\ell_1 + \dots + \ell_{W-1} + 1}), \dots, (\boldsymbol{a}^{\ell_1 + \dots + \ell_W}, b_{\ell_1 + \dots + \ell_W})\})$  in  $\mathbb{S}$  and **228** for any  $\boldsymbol{x} \in \Omega$ , by

$$Res_{S}(\boldsymbol{x}) = \sqrt{\sum_{i=1}^{\ell_{1}+\ldots+\ell_{W}} (b_{i} - \langle \boldsymbol{a}^{i}, \boldsymbol{x} \rangle)^{2}}.$$
(2)

Note that each element of this problem set S specifies an ordered sequence of W blocks of linear equations of the form  $\langle \boldsymbol{a}^i, \boldsymbol{x} \rangle = b_i$  where  $\langle *, * \rangle$  denotes the inner product in  $\mathbb{R}^J$ (and thus S is an appropriate representation of the so-called "ordered subsets" approach to tomographic reconstruction<sup>51</sup>, as well as of other earlier-published block-iterative methods that proposed essentially the same idea<sup>52-54</sup>). The proximity function *Res* on S is the *residual* that we get when a particular  $\boldsymbol{x}$  is substituted into all the equations of a particular problem S.

#### **B.** Algorithms and outputs

237 We now define the concept of an algorithm in the general context of problem structures. 238 For technical reasons that will become clear as we proceed with our development, we introduce an additional set  $\Delta$ , such that  $\Omega \subseteq \Delta \subseteq \mathbb{R}^J$ . (Both  $\Omega$  and  $\Delta$  are assumed to be known 239 and fixed for any particular problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$ .) An algorithm **P** for a problem 240 structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  assigns to each problem  $T \in \mathbb{T}$  an operator  $\mathbf{P}_T : \Delta \to \Omega$ . This definition is 241 used to define iterative processes that, for any *initial point*  $\boldsymbol{x} \in \Omega$ , produce the (potentially) 242 infinite sequence  $\left(\left(\mathbf{P}_{T}\right)^{k}\boldsymbol{x}\right)_{k=0}^{\infty}$  (that is, the sequence  $\boldsymbol{x}, \mathbf{P}_{T}\boldsymbol{x}, \mathbf{P}_{T}\left(\mathbf{P}_{T}\boldsymbol{x}\right), \cdots$ ) of points in 243  $\Omega$ . We discuss below how such a potentially infinite process is terminated in practice. 244

245 Selecting  $\Omega = \mathbb{R}^J_+$  and  $\Delta = \mathbb{R}^J$  for the problem structure  $\langle \mathbb{S}, Res \rangle$  of the previous subsec-246 tion, an example of an algorithm **R** is specified by

$$\mathbf{R}_{S}\boldsymbol{x} = \mathbf{Q}\mathbf{B}_{S_{W}}\cdots\mathbf{B}_{S_{1}}\boldsymbol{x},\tag{3}$$

**247** where S is the problem specified above (2) and, for  $1 \le w \le W$ ,  $\mathbf{B}_{S_w} : \Delta \to \Delta$  is defined by

$$\mathbf{B}_{S_w} \boldsymbol{x} = \boldsymbol{x} + \frac{1}{\ell_w} \sum_{i=\ell_1+\ldots+\ell_{w-1}+1}^{\ell_1+\ldots+\ell_w} \frac{b_i - \langle \boldsymbol{a}^i, \boldsymbol{x} \rangle}{\|\boldsymbol{a}^i\|^2} \boldsymbol{a}^i,$$
(4)

**248** where  $||\boldsymbol{a}||$  denotes the norm of the vector  $\boldsymbol{a}$  in  $\mathbb{R}^J$ , and  $\mathbf{Q}: \Delta \to \Omega$  is defined by

$$\left(\mathbf{Q}\boldsymbol{x}\right)_{j} = \max\left\{0, \boldsymbol{x}_{j}\right\}, \text{ for } 1 \le j \le J.$$
(5)

Note that  $\mathbf{R}_S : \Delta \to \Omega$ . This specific algorithm **R** is a typical example of the so-called block-249 iterative methods mentioned above. Except for the presence of  $\mathbf{Q}$  in (3), which enforces 250 nonnegativity of the components, it is identical to an algorithm used and illustrated  $in^{31}$ . 251 With the **Q** absent from the definition of the algorithm,  $\Omega$  has to be the whole of  $\mathbb{R}^{J}$ ; the 252 practical consequence of the presence versus the absence of  $\mathbf{Q}$  in the tomographic application 253 is illustrated in Subsection III D. We note also that special cases of the presented algorithm 254 include the classical reconstruction methods ART (if  $\ell_w = 1$ , for  $1 \le w \le W$ ) and SIRT (if 255 W = 1; see, for example, Chapters 11 and 12 of<sup>55</sup>. 256

For a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$ , a  $T \in \mathbb{T}$ , an  $\varepsilon \in \mathbb{R}_+$  and a sequence  $R = (\boldsymbol{x}^k)_{k=0}^{\infty}$ of points in  $\Omega$ , we use  $O(T, \varepsilon, R)$  to denote the  $\boldsymbol{x} \in \Omega$  that has the following properties:  $\mathcal{P}r_T(\boldsymbol{x}) \leq \varepsilon$  and there is a nonnegative integer K such that  $\boldsymbol{x}^K = \boldsymbol{x}$  and, for all nonnegative integers k < K,  $\mathcal{P}r_T(\boldsymbol{x}^k) > \varepsilon$ . Clearly, if there is such an  $\boldsymbol{x}$ , then it is unique. If there is no 261 such x, then we say that  $O(T, \varepsilon, R)$  is *undefined*, otherwise we say that it is *defined*. The 262 intuition behind this definition is the following: if we think of R as the (infinite) sequence of 263 points that is produced by an algorithm (intended for the problem T) without a termination 264 criterion, then  $O(T, \varepsilon, R)$  is the *output* produced by that algorithm when we add to it 265 instructions that make it terminate as soon as it reaches a point that is  $\varepsilon$ -compatible with 266 T.

267

## C. Bounded perturbation resilience

The notion of a bounded perturbations resilient algorithm  $\mathbf{P}$  for a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  has been defined in a mathematically precise manner<sup>29</sup>. However, that definition is not satisfactory from the point of view of applications in medical physics (or indeed in any area involving noisy data), because it is useful only for problems T for which there is a perfectly compatible solution (that is, an  $\boldsymbol{x}$  such that  $\mathcal{P}r_T(\boldsymbol{x}) = 0$ ). We therefore extend here that notion as follows. An algorithm  $\mathbf{P}$  for a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  is said to be strongly perturbation resilient if, for all  $T \in \mathbb{T}$ ,

275 (i) there exists an 
$$\varepsilon \in \mathbb{R}_+$$
 such that  $O\left(T, \varepsilon, \left(\left(\mathbf{P}_T\right)^k \boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined for every  $\boldsymbol{x} \in \Omega$ ;

276 (ii) for all  $\varepsilon \in \mathbb{R}_+$  such that  $O\left(T, \varepsilon, \left((\mathbf{P}_T)^k \boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined for every  $\boldsymbol{x} \in \Omega$ , we also 277 have that  $O\left(T, \varepsilon', R\right)$  is defined for every  $\varepsilon' > \varepsilon$  and for every sequence  $R = (\boldsymbol{x}^k)_{k=0}^{\infty}$ 278 of points in  $\Omega$  generated by

$$\boldsymbol{x}^{k+1} = \mathbf{P}_T \left( \boldsymbol{x}^k + \beta_k \boldsymbol{v}^k \right), \text{ for all } k \ge 0,$$
(6)

279 where  $\beta_k \boldsymbol{v}^k$  are bounded perturbations, meaning that the sequence  $(\beta_k)_{k=0}^{\infty}$  of nonnega-280 tive real numbers is summable (that is,  $\sum_{k=0}^{\infty} \beta_k < \infty$ ), the sequence  $(\boldsymbol{v}^k)_{k=0}^{\infty}$  of vectors 281 in  $\mathbb{R}^J$  is bounded and, for all  $k \ge 0$ ,  $\boldsymbol{x}^k + \beta_k \boldsymbol{v}^k \in \Delta$ .

In less formal terms, the second of these properties says that for a strongly perturbation resilient algorithm we have that, for every problem and any nonnegative real number  $\varepsilon$ , if it is the case that for all initial points from  $\Omega$  the infinite sequence produced by the algorithm contains an  $\varepsilon$ -compatible point, then it will also be the case that all perturbed sequences satisfying (6) contain an  $\varepsilon'$ -compatible point, for any  $\varepsilon' > \varepsilon$ . 287 Having defined the notion of a strongly perturbation resilient algorithm, we next show 288 that this notion is of relevance to problems in medical physics. We illustrate the use of this 289 in tomography in the next section. We first need to introduce some mathematical concepts. Given an algorithm **P** for a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  and a  $T \in \mathbb{T}$ , we say that 290 **P** is convergent for T if, for every  $\boldsymbol{x} \in \Omega$ , there exists a unique  $\boldsymbol{y}(\boldsymbol{x}) \in \Omega$  such that, 291  $\lim_{k\to\infty} \left(\mathbf{P}_T\right)^k \boldsymbol{x} = \boldsymbol{y}\left(\boldsymbol{x}\right)$ , meaning that for every positive real number  $\delta$ , there exist a non-292 negative integer K, such that  $\left\| \left( \mathbf{P}_T \right)^k \boldsymbol{x} - \boldsymbol{y} \left( \boldsymbol{x} \right) \right\| \leq \delta$ , for all nonnegative integers  $k \geq K$ . 293 If, in addition, there exists a  $\gamma \in \mathbb{R}_+$  such that  $\mathcal{P}r_T(\boldsymbol{y}(\boldsymbol{x})) \leq \gamma$ , for every  $\boldsymbol{x} \in \Omega$ , then we 294 295 say that  $\mathbf{P}$  is boundedly convergent for T.

A function  $f: \Omega \to \mathbb{R}$  is uniformly continuous if, for every  $\varepsilon > 0$  there exists a  $\delta > 0$ , such that, for all  $x, y \in \Omega$ ,  $|f(x) - f(y)| \le \varepsilon$  provided that  $||x - y|| \le \delta$ . An example of a uniformly continuous function is  $\operatorname{Res}_S$  of (2), for any  $S \in S$ . This can be proved by observing that the right-hand side of (2) can be rewritten in vector/matrix form as ||b - Ax|| and then selecting, for any given  $\varepsilon > 0$ ,  $\delta$  to be  $\varepsilon / ||A||$ , where ||A|| denotes the matrix norm of **301** A.

An operator  $\mathbf{O} : \Delta \to \Omega$ , is *nonexpansive* if  $\|\mathbf{O}\boldsymbol{x} - \mathbf{O}\boldsymbol{y}\| \leq \|\boldsymbol{x} - \boldsymbol{y}\|$ , for all  $\boldsymbol{x}, \boldsymbol{y} \in \Delta$ . 303 An example of a nonexpansive operator is the  $\mathbf{R}_S$  of (3). The proof of this is also simple. 304 It follows from discussions regarding similar claims in<sup>27</sup> that the  $\mathbf{B}_{S_w} : \mathbb{R}^J \to \mathbb{R}^J$  of (4) is a 305 nonexpansive operator, for  $1 \leq w \leq W$ , and that the operator  $\mathbf{Q}$  of (5) is also nonexpansive. 306 Obviously, a sequential application of nonexpansive operators results in a nonexpansive 307 operator and thus  $\mathbf{R}_S$  is nonexpansive.

308 Now we state an important new result that gives sufficient conditions for strong perturbation resilience: If P is an algorithm for a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  such that, 309 for all  $T \in \mathbb{T}$ ,  $\mathbf{P}$  is boundedly convergent for T,  $\mathcal{P}r_T : \Omega \to \mathbb{R}$  is uniformly 310 continuous and  $\mathbf{P}_T:\Delta 
ightarrow \Omega$  is nonexpansive, then  $\mathbf{P}$  is strongly perturbation 311 resilient. The importance of this result lies in the fact that the rather ordinary condition 312 313 of uniform continuity for the proximity function and the reasonable conditions of bounded convergence and nonexpansiveness of the algorithmic operators guarantee that we end up 314 315 with a strongly perturbation resilient algorithm. The proof of this new result involves some mathematical technicalities and is therefore presented in the Appendix as Theorem 1. 316

## D. Optimization criterion and nonascending vector

318 Now suppose, as is indeed the case for the constrained optimization problems discussed in the previous section, that in addition to a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  we are also provided 319 with an optimization criterion, which is specified by a function  $\phi : \Delta \to \mathbb{R}$ , with the 320 convention that a point in  $\Delta$  for which the value of  $\phi$  is smaller is considered superior (from 321 the point of view of our application) to a point in  $\Delta$  for which the value of  $\phi$  is larger. In the 322 tomography context, any of the functions of  $\boldsymbol{x}$  that are listed as a "secondary optimization" 323 criterion" (an alternative name is a "regularizer") in Section 6.4  $of^{55}$  is an acceptable choice 324 for the optimization criterion  $\phi$ . These include weighted norms, the negative of Shannon's 325 326 entropy and total variation. It is the last of these that we discuss in detail in the illustrative 327 example below. The essential idea of the superiorization methodology presented in this paper is to make use of the perturbations of (6) to transform a strongly perturbation resilient 328 algorithm that seeks a constraints-compatible solution into one whose outputs are equally 329 good from the point of view of constraints-compatibility, but are superior according to the 330 optimization criterion. We do this by producing from the algorithm another one, called its 331 superiorized version, by making sure not only that the  $\beta_k v^k$  are bounded perturbations, but 332 also that  $\phi\left(\boldsymbol{x}^{k}+\beta_{k}\boldsymbol{v}^{k}\right)\leq\phi\left(\boldsymbol{x}^{k}\right)$ , for all  $k\geq0$ . 333

In order to ensure this we introduce a new concept (closely related to the concept of a "descent direction" that is widely used in optimization). Given a function  $\phi : \Delta \to \mathbb{R}$  and a point  $\boldsymbol{x} \in \Delta$ , we say that a vector  $\boldsymbol{d} \in \mathbb{R}^J$  is *nonascending* for  $\phi$  at  $\boldsymbol{x}$  if  $\|\boldsymbol{d}\| \leq 1$  and

there is a 
$$\delta > 0$$
 such that for all  $\lambda \in [0, \delta]$ ,  
 $(\boldsymbol{x} + \lambda \boldsymbol{d}) \in \Delta \text{ and } \phi (\boldsymbol{x} + \lambda \boldsymbol{d}) \leq \phi (\boldsymbol{x}).$ 
(7)

337 Note that irrespective of the choices of  $\phi$  and x, there is always at least one nonascending vector d for  $\phi$  at x, namely the zero-vector, all of whose components are zero. This is a useful 338 339 fact for proving results concerning the guaranteed behavior of our proposed procedures. However, in order to steer our algorithms toward a point at which the value of  $\phi$  is small, 340 we need to find a d such that  $\phi(\boldsymbol{x} + \lambda \boldsymbol{d}) < \phi(\boldsymbol{x})$  rather than just  $\phi(\boldsymbol{x} + \lambda \boldsymbol{d}) \le \phi(\boldsymbol{x})$  as in 341 (7). In some earlier papers on superiorization<sup>27-31</sup> it was assumed that  $\Delta = \mathbb{R}^J$  and that  $\phi$ 342 is a convex function. This implied that, for any point  $\boldsymbol{x} \in \Delta$ ,  $\phi$  had a subgradient  $\boldsymbol{g} \in \mathbb{R}^J$  at 343 the point  $\boldsymbol{x}$ . It was suggested that if there is such a  $\boldsymbol{g}$  with a positive norm, then  $\boldsymbol{d}$  should 344 be chosen to be -g/||g||, otherwise d should be chosen to be the zero vector. However, 345

346 there are approaches (not involving subgradients) to selecting an appropriate d; an example 347 can be found in<sup>32</sup> in which d is found without using subgradients for the case when  $\phi$  is the 348  $\ell_1$ -norm of the Haar transform. The method we used for selecting a nonascending vector in 349 the experiments reported in this paper is specified at the end of Subsection III A.

350

# E. Superiorized version of an algorithm

351 We now make precise the ingredients needed for transforming an algorithm into its superiorized version. Let  $\Omega$  and  $\Delta$  be the underlying sets for a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$ 352  $(\Omega \subseteq \Delta \subseteq \mathbb{R}^J$ , as discussed at the beginning of Subsection IIB), **P** be an algorithm for 353  $\langle \mathbb{T}, \mathcal{P}r \rangle$  and  $\phi : \Delta \to \mathbb{R}$ . The following description of the Superiorized Version of Algorithm 354 **P** produces, for any problem  $T \in \mathbb{T}$ , a sequence  $R_T = (\boldsymbol{x}^k)_{k=0}^{\infty}$  of points in  $\Omega$  for which, for 355 all  $k \ge 0$ , (6) is satisfied. We show this to be true, for any algorithm **P**, after the description 356 of the Superiorized Version of Algorithm **P**. Furthermore, since the sequence  $R_T$  is steered 357 358 by Superiorized Version of Algorithm **P** toward a reduced value of  $\phi$ , there is an intuitive expectation that the output of the superiorized version is likely to be superior (from the 359 point of view of the optimization criterion  $\phi$ ) to the output of the original unperturbed 360 algorithm. This last statement is not precise and so it cannot be proved in a mathematical 361 sense for an arbitrary algorithm  $\mathbf{P}$ ; however, that should not stop us from applying the 362 easy procedure given below for automatically producing the Superiorized Version of  $\mathbf{P}$  and 363 experimentally checking whether it indeed provides us with outputs superior to those of the 364 365 original algorithm. The well-demonstrated nature of heuristic optimization approaches is that they often work in practice even when their performance cannot be guaranteed to be 366 optimal<sup>33-35</sup>. 367

368 Nevertheless, we can push our theory further than the hope expressed in the last paragraph, by considering superiorized versions of algorithms that satisfy some condition. In 369 370 this paper, the condition that we discuss is strong perturbation resilience. We show below that if **P** is strongly perturbation resilient, then, for any problem  $T \in \mathbb{T}$ , a sequence  $R_T$ 371 produced by its superiorized version has the following desirable property: For all  $\varepsilon \in \mathbb{R}_+$ , if 372  $O\left(T,\varepsilon,\left(\left(\mathbf{P}_{T}\right)^{k}\boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined for every  $\boldsymbol{x}\in\Omega$ , then  $O\left(T,\varepsilon',R_{T}\right)$  is also defined for every 373  $\varepsilon' > \varepsilon$ ; in other words, the Superiorized Version of Algorithm **P** provides an  $\varepsilon'$ -compatible 374 375 output. As stated above, the advantage of the superiorized version is that its output is 376 likely to be superior to the output of the original unperturbed algorithm. We point out that 377 strong perturbation resilience is a sufficient, but not necessary, condition for guaranteeing 378 such desirable behavior of the superiorized version, finding additional sufficient conditions 379 and proving that algorithms that we wish to superiorize satisfy such conditions is part of 380 our ongoing research.

The superiorized version assumes that we have available a summable sequence  $(\gamma_{\ell})_{\ell=0}^{\infty}$  of positive real numbers (for example,  $\gamma_{\ell} = a^{\ell}$ , where 0 < a < 1) and it generates, simultaneously with the sequence  $(\boldsymbol{x}^k)_{k=0}^{\infty}$ , sequences  $(\boldsymbol{v}^k)_{k=0}^{\infty}$  and  $(\beta_k)_{k=0}^{\infty}$ . The latter is generated as a subsequence of  $(\gamma_{\ell})_{\ell=0}^{\infty}$ , resulting in a summable sequence  $(\beta_k)_{k=0}^{\infty}$ . The algorithm further depends on a specified initial point  $\bar{\boldsymbol{x}} \in \Omega$  and on a positive integer N. It makes use of a logical variable called *loop*.

387 Superiorized Version of Algorithm P

- **388** (i) set k = 0
- 389 (ii) set  $x^k = \bar{x}$
- **390** (iii) set  $\ell = -1$
- **391** (iv) repeat
- **392** (v) **set** n = 0
- **393** (vi) **set**  $x^{k,n} = x^k$
- **394** (vii) **while** n < N
- **395** (viii) **set**  $\boldsymbol{v}^{k,n}$  to be a nonascending vector for  $\phi$  at  $\boldsymbol{x}^{k,n}$
- **396** (ix) set loop=true
- **397** (x) **while** *loop*
- **398** (xi) **set**  $\ell = \ell + 1$
- **399** (xii) **set**  $\beta_{k,n} = \gamma_{\ell}$
- **400** (xiii) set  $z = x^{k,n} + \beta_{k,n} v^{k,n}$
- 401 (xiv) if  $z \in \Delta$  and  $\phi(z) \le \phi(x^k)$  then

- **402** (xv) set n = n + 1
- **403** (xvi) set  $x^{k,n} = z$

**404** (xvii) set loop = false

- 405 (xviii) set  $\boldsymbol{x}^{k+1} = \mathbf{P}_T \boldsymbol{x}^{k,N}$
- **406** (xix) **set** k = k + 1

407 Next we analyze the behavior of the Superiorized Version of Algorithm P.

The iteration number k is set to 0 in (i) and  $\mathbf{x}^k = \mathbf{x}^0$  is set to its initial value  $\bar{\mathbf{x}}$  in (ii). The 408 integer index  $\ell$  for picking the next element from the sequence  $(\gamma_{\ell})_{\ell=0}^{\infty}$  is initialized to -1 by 409 line (iii), it is repeatedly increased by line (xi). The lines (v) - (xix) that follow the **repeat** 410 in (iv) perform a complete iterative step from  $\boldsymbol{x}^k$  to  $\boldsymbol{x}^{k+1}$ , infinite repetitions of such steps 411 provide the sequence  $R_T = (\boldsymbol{x}^k)_{k=0}^{\infty}$ . During one iterative step, there is one application of 412 the operator  $\mathbf{P}_T$ , in line (xviii), but there are N steering steps aimed at reducing the value of 413  $\phi$ ; the latter are done by lines (v) - (xvii). These lines produce a sequence of points 414  $oldsymbol{x}^{k,n}$ , where  $0\leq n\leq N$  with  $oldsymbol{x}^{k,0}=oldsymbol{x}^k$ ,  $oldsymbol{x}^{k,n}\in\Delta$  and  $\phi\left(oldsymbol{x}^{k,n}
ight)\leq\phi\left(oldsymbol{x}^k
ight).$ 415

We prove the truth of the last sentence by induction on the nonnegative integers. For 416 n = 0, we have by lines (v) and (vi) that  $\boldsymbol{x}^{k,0} = \boldsymbol{x}^k$ . But  $\boldsymbol{x}^k \in \Omega$ , since it is either  $\bar{\boldsymbol{x}}$  that is 417 assumed to be in  $\Omega$  due to lines (i) and (ii) or it is in the range  $\Omega$  of  $\mathbf{P}_T$  due to lines (xviii) 418 and (xix). Now we assume, for any  $0 \le n < N$ , that  $\boldsymbol{x}^{k,n} \in \Delta$  and  $\phi(\boldsymbol{x}^{k,n}) \le \phi(\boldsymbol{x}^k)$  and 419 show that lines (viii) - (xvii) perform a computation that leads from  $\boldsymbol{x}^{k,n}$  to an  $\boldsymbol{x}^{k,n+1} \in \Delta$ 420 that satisfies  $\phi(x^{k,n+1}) \leq \phi(x^k)$ . To see this, observe that line (viii) sets  $v^{k,n}$  to be a 421 nonascending vector for  $\phi$  at  $\boldsymbol{x}^{k,n}$ , which implies that (7) is satisfied with  $\boldsymbol{x} = \boldsymbol{x}^{k,n}$  and 422  $d = v^{k,n}$ . Line (ix) sets *loop* to *true*, and it remains *true* while searching for the desired 423  $\boldsymbol{x}^{k,n+1}$ , by repeatedly executing the loop sequence that follows line (x). In this sequence, 424 line (xi) increases  $\ell$  by 1 and line (xii) sets  $\beta_{k,n}$  to  $\gamma_{\ell}$ . Thus for the vector  $\boldsymbol{z}$  defined by line 425 (xiii),  $\boldsymbol{z} \in \Delta$  and  $\phi(\boldsymbol{z}) \leq \phi(\boldsymbol{x}^{k,n})$ , provided that  $\beta_{k,n}$  is not greater than the  $\delta$  in (7). Since 426  $(\gamma_\ell)_{\ell=0}^\infty$  is a summable sequence of positive real numbers, there must be a positive integer L 427 such that  $\gamma_{\ell} \leq \delta$ , for all  $\ell \geq L$ . This implies that if we applied lines (xi) - (xiii) often enough, 428 we would reach a vector  $\boldsymbol{z}$  that satisfies  $\boldsymbol{z} \in \Delta$  and  $\phi(\boldsymbol{z}) \leq \phi(\boldsymbol{x}^{k,n})$ . If the condition in line 429 430 (xiv) is not satisfied when the process gets to it, then lines (xi) - (xiii) are again executed and eventually we get a vector  $\boldsymbol{z}$  for which the condition in line (xiv) is satisfied due to the 431

induction hypothesis that  $\phi(\mathbf{x}^{k,n}) \leq \phi(\mathbf{x}^k)$ . By lines (xv) and (xvi) we see that at that 432 time  $\boldsymbol{x}^{k,n+1}$  is set to  $\boldsymbol{z}$  and so we obtain that  $\boldsymbol{x}^{k,n+1} \in \Delta$  and  $\phi(\boldsymbol{x}^{k,n+1}) \leq \phi(\boldsymbol{x}^k)$ , as desired. 433 Line (xvii) sets loop to false and so control is returned to line (vii). When this happens for 434 the Nth time, it will be the case that n = N and therefore line (xviii) is used to produce 435  $\boldsymbol{x}^{k+1} \in \Omega$  and the increasing of k by line (xix) allows us then to move on to the next iterative 436 step. Infinite repetition of such steps produces the sequence  $R_T = (\boldsymbol{x}^k)_{k=0}^{\infty}$  of points in  $\Omega$ . 437 We now show that if  $O\left(T,\varepsilon,\left(\left(\mathbf{P}_{T}\right)^{k}\boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined for every  $\boldsymbol{x} \in \Omega$ , then, for any 438  $\varepsilon' > \varepsilon$ , the Superiorized Version of Algorithm **P** produces an  $\varepsilon'$ -compatible output. Since **P** 439 is assumed to be strongly perturbation resilient, this desired result follows if we can show 440 that there exists a summable sequence  $(\beta_k)_{k=0}^{\infty}$  of nonnegative real numbers and a bounded 441 sequence  $(\boldsymbol{v}^k)_{k=0}^{\infty}$  of vectors in  $\mathbb{R}^J$  such that (6) is satisfied for all  $k \geq 0$ . In view of line 442 (xviii), this is achieved if we can define the  $\beta_k$  and the  $v^k$  so that  $x^{k,N} = x^k + \beta_k v^k$ . This 443 444 is done by setting

$$\beta_k = \max\left\{\beta_{k,n} \,|\, 0 \le n < N\right\},\tag{8}$$

$$\boldsymbol{v}^{k} = \sum_{n=0}^{N-1} \frac{\beta_{k,n}}{\beta_{k}} \boldsymbol{v}^{k,n}.$$
(9)

445 That these assignments result in  $\boldsymbol{x}^{k,N} = \boldsymbol{x}^k + \beta_k \boldsymbol{v}^k$  follows from lines (v) - (xvii). From line 446 (xii) follows that  $(\beta_k)_{k=0}^{\infty}$  is a subsequence of  $(\gamma_\ell)_{\ell=0}^{\infty}$  and, hence, it is a summable sequence 447 of nonnegative real numbers. Since each  $\|\boldsymbol{v}^{k,n}\| \leq 1$  by the definition of a nonascending 448 vector, it follows from (8) and (9) that  $\|\boldsymbol{v}^k\| \leq N$  and so  $(\boldsymbol{v}^k)_{k=0}^{\infty}$  is bounded. Part of the 449 condition expressed in (6) is that, for all  $k \geq 0$ ,  $\boldsymbol{x}^k + \beta_k \boldsymbol{v}^k \in \Delta$ . This follows from the fact 450 that  $\boldsymbol{x}^{k,N} = \boldsymbol{x}^k + \beta_k \boldsymbol{v}^k$  is assigned its value by line (xvi), but only if the condition expressed 451 in line (xiv) is satisfied.

In conclusion, we have shown that the superiorized version of a strongly perturbation resilient algorithm produces outputs that are essentially as constraints-compatible as those produced by the original version of the algorithm. However, due to the repeated steering of the process by lines (vii) - (xvii) toward reducing the value of the optimization criterion  $\phi$ , we can expect that the output of the superiorized version will be superior (from the point of view of  $\phi$ ) to the output of the original algorithm.

## F. Information on performance comparison with MAP methods

459 Using our notation, the constrained minimization formulation that we are considering is:
460 Given an ε ∈ ℝ<sub>+</sub>,

minimize 
$$\phi(\boldsymbol{x})$$
, subject to  $\mathcal{P}r_T(\boldsymbol{x}) \leq \varepsilon$ . (10)

The aim of superiorization is not identical with the aim of constrained minimization in (10). 461 One difference is that  $\varepsilon$  is not "given" in the superiorization context. The superiorization 462 463 of an algorithm produces a sequence and, for any  $\varepsilon$ , the associated output of the algorithm is considered to be the first  $\boldsymbol{x}$  in the sequence for which  $\mathcal{P}r_T(\boldsymbol{x}) \leq \varepsilon$ . The other difference 464 is that we do not claim that this output is a minimizer of  $\phi$  among all points that satisfy 465 the constraint, but hope only that it is usually an  $\boldsymbol{x}$  for which  $\phi(\boldsymbol{x})$  is at the small end 466 467 of its range of values over the set of constraint-satisfying points. This latter difference is 468 generally shared by comparisons of a heuristic approach with an exact approach to solving a constrained minimization problem. 469

470 The MAP (or regularized) formulation of a physical problem that leads to the constrained 471 minimization problem (10) is the unconstrained minimization problem of the form: Given 472  $a \beta \in \mathbb{R}_+$ ,

minimize 
$$\left[\phi(\boldsymbol{x}) + \beta \mathcal{P} r_T(\boldsymbol{x})\right]$$
. (11)

473 Formulations of both kinds (i.e, the ones of (10) and of (11)) are widely used for solving 474 medical physics problems and the question "Which of these two formulations leads to faster or 475 better solutions of the underlying physical problem?" is open. Examples of both formulations 476 with various choices for  $\mathcal{P}r_T$  and  $\phi$  are listed in the beginning parts of the paper of Goldstein 477 and Osher<sup>47</sup>.

478 We now return to the question raised near the end of Section I: Will superiorization produce superior results to those produced by contemporary MAP methods or is it faster than 479 the better of such methods? As yet, there is very little information available regarding this 480 general question; in fact, we are aware of only one published study<sup>45</sup>. That study compared 481 a superiorization algorithm with the algorithm of Goldstein and Osher that they refer to 482 as TwIST<sup>46</sup> with split Bregman<sup>47</sup> as the substep, which is indeed a contemporary method 483 that uses the MAP formulation. (For example, see the discussion of the split Bregman 484 method in<sup>56</sup>.) The problem S to which the two algorithms were applied was one from the 485 tomographic problem set S defined in (1).  $Res_S$  as defined in (2) was used as the proximity 486

487 function and total variation, TV as defined below in (12), was the choice for  $\phi$ . It is reported 488 in<sup>45</sup> that for the outputs of the two algorithms that were being compared, the values of  $Res_S$ 489 and TV were very similar, but the superiorization algorithm produced its output four times 490 faster than the MAP method.

491

# **III. AN ILLUSTRATIVE EXAMPLE**

492

## A. Application to tomography

493 We use *tomography* to refer to the process of reconstructing a function over a Euclidean space from estimated values of its integrals along lines (that are usually, but not necessarily, 494 straight). The particular reconstruction processes to which our discussion applies are the 495 series expansion methods, see Section 6.3  $of^{55}$ , in which it is assumed that the function to 496 be reconstructed can be approximated by a linear combination of a finite number (say J) 497 498 of basis functions and the reconstruction task becomes one of estimating the coefficients of 499 the basis functions in the expansion. Sometimes, prior knowledge about the nature of the function to be reconstructed allows us to confine the sought-after vector  $\boldsymbol{x}$  of coefficients to 500 a subset  $\Omega$  of  $\mathbb{R}^J$  (such as the nonnegative orthant  $\mathbb{R}^J_+$ ). We use *i* to index the lines along 501 which we integrate,  $a^i \in \mathbb{R}^J$  to denote the vector whose *j*th component is the integral of the 502 *j*th basis function along the *i*th line, and  $b_i$  to denote the measured integral of the function 503 504 to be reconstructed along the *i*th line. Under these circumstances the constraints come from the desire that, for each of the lines,  $\langle a^i, x \rangle$  should be close (in some sense) to  $b_i$ . 505

To make this concrete, consider (1). Such a description of the constraints arises in tomography by grouping the lines of integration into W blocks, with  $\ell_w$  lines in the wth block. Such groupings often (but not always) are done according to some geometrical condition on the lines (for example, in case of straight lines, we may decide that all the lines that are parallel to each other form one block). In this framework the proximity function *Res* defined by (2) provides a reasonable measure of the incompatibility of a vector  $\boldsymbol{x}$  with the constraints. The algorithm **R** described by (3) - (5) is applicable to this concrete formulation.

**513** There are many optimization criteria that have been used in tomography, see Section **514** 6.4 of<sup>55</sup>, here we discuss the one called *total variation* (TV), whose use has been popular **515** in medical physics recently, see as examples<sup>20,22,23,41-44</sup>. The definition of TV that we use 516 here requires a certain way of selecting the basis functions. It is assumed that the function to be reconstructed is defined in the plane  $\mathbb{R}^2$  and is zero-valued outside a square-shaped 517 region in the plane. This region is subdivided into J smaller equal-sized squares (*pixels*) 518 and the J basis functions are defined by having value one in exactly one pixel and value 519 zero everywhere else. We index the pixels by j and we let C denote the set of all indices of 520 pixels that are not in the rightmost column or the bottom row of the pixel array. For any 521 pixel with index j in C, let r(j) and b(j) be the index of the pixel to its right and below it, 522 respectively. We define  $TV : \mathbb{R}^J \to \mathbb{R}$  by 523

$$TV(\boldsymbol{x}) = \sum_{j \in C} \sqrt{\left(x_j - x_{r(j)}\right)^2 + \left(x_j - x_{b(j)}\right)^2}.$$
 (12)

524 The method we adopted to generate a nonascending vector for the TV function at an  $\boldsymbol{x} \in \mathbb{R}^J$  is based on Theorem 2 of the Appendix. It is applicable since  $TV : \mathbb{R}^J \to \mathbb{R}$  is a 525 convex function; see, for example, the end of the Proof of Proposition 1  $of^{41}$ . Now consider 526 an integer j' such that  $1 \leq j' \leq J$ . Looking at the sum in (12), we see that  $x_{j'}$  appears in 527 at most three terms, in which j' must be either j, or r(j), or b(j) for some  $j \in C$ . By taking 528 the formal partial derivatives of these three terms, we see that  $\frac{\partial TV}{\partial x_{i'}}(\boldsymbol{x})$  is well-defined if the 529 denominator in the formal derivative of any of the three terms is not zero for  $\boldsymbol{x}$ . In view of 530 531 this, we define the g in Theorem 2 as follows. If the denominator in any of the three formal partial derivatives with respect to  $x_{i'}$  has an absolute value less than a very small positive 532 number (we used  $10^{-20}$  ), then we set  $g_{j'}$  to zero, otherwise we set it to  $\frac{\partial TV}{\partial x_{j'}}(\boldsymbol{x})$ . Clearly 533 the resulting  $\boldsymbol{g} \in \mathbb{R}^J$  satisfies the condition in Theorem 2 and hence provides a  $\boldsymbol{d}$  that is a 534 nonascending vector for TV at  $\boldsymbol{x}$ . 535

Previously reported reconstructions using TV-superiorization selected the d using subformation gradients as discussed in the paragraph following (7); such a d is not guaranteed to be a nonascending vector for the TV function. What we are proposing here is not only mathematically rigorous (in the sense that it is guaranteed to produce a nonascending vector for the TV function), but it can also lead to a better reconstructions, as illustrated in Subsection III D. 546

#### В. The data generation for the experiments

543 The data sets used in the experiments reported in this paper were generated in such a way that they share the noise-characteristics of CT scanners when used for scanning the 544 human head and brain; as discussed, for example, in Chapter 5 of  $^{55}$ . They were generated 545 using the software SNARK09<sup>57</sup>.

547 The head phantom that was used for data generation is based on an actual cross-section of the human head. It is described as a collection of geometrical objects (such as ellipses, 548 triangles and segments of circles) whose combination accurately resembles the anatomical 549 550 features of the actual head cross-section. In addition, the basic phantom contains a large 551 tumor. The actual phantom used was obtained by a random variation of the basic phantom, 552 by incorporating into it local inhomogeneities and small low-contrast tumors at random locations. This phantom is represented by the image in figure 1. That image comprises 553 554  $485 \times 485$  pixels each of size 0.376 mm by 0.376 mm. The values assigned to the pixels are 555 obtained by an  $11 \times 11$  sub-sampling of the pixels and averaging the values assigned to the sub-samples by the geometrical objects that are used to describe the anatomical features 556 and the tumors. Those values are approximate linear attenuation coefficients per cm at 60 557 558 keV (0.416 for bone, 0.210 for brain, 0.207 for cerebrospinal fluid). The contrast of the small tumors with their background is 0.003 cm<sup>-1</sup>. In order to clearly see the low-contrast details 559 in the interior of the skull, we use zero (black) to represent the value 0.204 (or anything 560 less) and 255 (white) to represent 0.21675 or anything more). The same is true for all the 561 images in the rest of this paper, with the exception of those in figure ??. 562

563 For the selected head phantom we generated *parallel projection data*, in which one view comprises estimates of integrals through the phantom for a set of 693 equally-spaced parallel 564 lines with a spacing of 0.0376 cm between them. (We chose to simulate parallel rather 565 than divergent projection data, since the reconstruction by the method of<sup>42</sup> with which 566 we wish to compare the superiorization approach were performed for us by the authors 567  $of^{42}$  on parallel data. Even though contemporary CT scanners use divergent projection 568 data, results obtained by the use of parallel projection data are relevant to them, since it 569 is known that the quality of reconstructions from these two modes of data collection are 570 very similar as long as the data generations use similar frequencies of sampling of lines and 571 similar noise characteristics in the estimated integrals for those lines; see, for example, the 572



Figure 1: (a) A head phantom. (b) Reconstruction of the head phantom from realistically simulated projection data for 360 views using ART with blob basis functions.

reconstructions from divergent and parallel projection data in figure 5.15 of  $^{55}$ .) In calculating 573 574 these estimates we take into consideration the effects of photon statistics, detector width and scatter. Details of how we do this exactly can be found in Sections 5.5 and 5.9 of  $5^{5_5}$ . 575 576 Briefly, quantum noise is calculated based on the assumption that approximately 2,000,000 photons enter the head along each ray, detector width is simulated by using 11 sub-rays 577 along each of which the attenuation is calculated independently and then combined at the 578 detector, and 5% of the photons get counted not by the detector for the ray in question but 579 detectors for the neighboring rays. For the experiments in this paper, we did not simulate 580 581 the poly-energetic nature of the x-ray source. To indicate what can be achieved in clinical CT, we show in figure 1(b) a reconstruction that was made from data comprising of 360 582 583 such views with the reconstruction algorithm known as ART with blob basis functions; see<sup>55</sup> (Chapter 11). 584

## C. Superiorization reconstruction from a few views

The main reason in the literature for advocating the use of TV as the optimization criterion is that by doing so one can achieve efficacious reconstructions even from sparsely sampled data. In our own work<sup>31</sup> with realistically simulated CT data we found that this is not always the case and this will be demonstrated again by the experiments reported in the current paper.

There have appeared in the literature some approaches to TV minimization that seem 591 to indicate a more efficacious performance for CT than the one reported in<sup>31</sup>. One of these 592 is the Adaptive Steepest Descent Projections Onto Convex Sets (ASD-POCS) algorithm, 593 which is described in detail in the much-cited paper of Sidky and Pan<sup>42</sup> and whose use has 594 been since reported in a number of subsequent publications, for example,  $in^{23,43}$ . We note 595 that ASD-POCS was designed with the aim of producing an exact minimization algorithm, 596 in contrast to our heuristic superiorization approach. Translating equations (6)-(8) of  $^{42}$ 597 into our terminology, the aim of ASD-POCS is the following: Given an  $\varepsilon \in \mathbb{R}_+$ , find an 598  $\varepsilon$ -compatible  $\boldsymbol{x} \in \Omega = \mathbb{R}^J_+$  for which  $TV(\boldsymbol{x})$  is minimal. (Note that this aim is a special 599 case of the constrained optimization formulation presented in (10).) In order to test ASD-600 601 POCS, we generated realistic projection data as described in the previous subsection but for only 60 views at 3 degree increments with the spacing between the lines for which 602 integrals are estimated set at 0.752 mm. Thus the number of rays (and hence the number 603 photons put into the head) in this data set is a twelfth of what it is in the data set used to 604 produce the reconstruction in figure 1(b). A reconstruction from these data was produced 605 for us using ASD-POCS by the authors of  $^{42}$  (this ensured that it does not suffer due to our 606 misinterpretation of the algorithm or from our inappropriate choices of the free parameters), 607 it is shown in figure 2(a). 608

Since the image quality of figure 2(a) is not anywhere near to that of figure 1(b), we present here a brief discussion as to why we are showing such images. Many publications in the recent medical imaging literature have claimed that medically-efficacious reconstructions can be obtained by the use of TV-minimization from data as sparse as what was used to produce figure 2(a). (In fact, ASD-POCS was motivated and used with such an aim in mind<sup>23,42,43</sup>.) Such publications usually show reconstructions from sparse data as evidence for the validity of their claims. They can do this because in their presented illustrations the features that



Figure 2: Reconstructions using TV as the optimization criterion from realistically simulated projection data for 60 views using (a) ASD-POCS and (b) superiorization. As compared to figure 1(b), these reconstructions fail in two ways: they do not show some of the fine details in the phantom and they present some artifactual variations. The former of these is a consequence of reconstructing from a much smaller data set than used for figure 1(b). The latter is due to using a very narrow window (13.5 HU) in these displays. Were we to use a wider display window (e.g., from -429 HU to 429 HU) for the reconstructions in this figure and in figure 1(b), the visual appearance of the resulting images would be nearly indistinguishable.

are observable in the reconstructions are usually much larger and/or of much higher contrast 616 617 against their backgrounds than the small "tumors" in figure 1(a), which are perfectly visible 618 in the reconstruction in figure 1(b), but are not detectable in the reconstruction from sparse 619 data in figure 2(a). The reason why that reconstruction appears to be unacceptably bad is that the display window (from  $0.204 \text{ cm}^{-1}$  linear attenuation coefficient to  $0.21675 \text{ cm}^{-1}$  linear 620 attenuation coefficient) is very narrow; it was selected to enhance the visibility of the small 621 622 low-contrast tumors. The width of this window corresponds to about 13.5 Hounsfield Units (HU). As compared to this, in their evaluation of sparse-view reconstruction from flat-panel-623 detector cone-beam CT, Bian et al.<sup>43</sup> use what they call a "soft-tissue grayscale window" 624

625 (also a "narrow window") from -429 HU to 429 HU to display head phantom reconstructions. 626 Using such a window for our reconstructions shown figures 2(a) and 1(b) would result in images that are nearly indistinguishable from each other. Thus reporting the images using 627 such a display window is consistent with the claim that a TV-minimizing reconstruction 628 from a few views is similar in quality to a more traditional reconstruction from many views. 629 However, our much narrower display window reveals that this is not really so. We therefore 630 continue using our much narrower window in what follows, since it clearly reveals the nature 631 632 of the reconstructions being compared, warts and all.

633 While this ASD-POCS reconstruction is not as good as it should be for diagnostic CT of
634 the brain (due to the sparsity of the data), it is visually better than the reconstruction using
635 superiorization from similar data as reported in<sup>31</sup>. We discuss the reasons for this in the
636 next subsection. Here we concentrate on examining whether one can achieve a reconstruction
637 using superiorization that is as good as that produced by ASD-POCS from the same data.

For this we first need to examine the numerical properties of the ASD-POCS reconstruc-639 tion. This reconstruction uses  $485 \times 485$  pixels each of size 0.376 mm by 0.376 mm. This 640 implies that J = 235, 225 and it also determines the components of the vectors  $a^i \in \mathbb{R}^J$  in 641 the precise specification of the problem S. The  $Res_S$ , as defined by (2), of the ASD-POCS 642 reconstruction is 0.33 and the TV, as defined by (12), is 835.

We applied to the same problem S a superiorized version of the algorithm  $\mathbf{R}$  defined 643 644 by (3). To complete the specification of **R**, we point out that for the ordering of views we chose the "efficient" one that was introduced in<sup>58</sup> and is also discussed on page 209 of<sup>55</sup>. 645 The choices we made for the superiorization are the following:  $\gamma_{\ell} = 0.99995^{\ell}, \, \bar{x}$  is the zero 646 vector and N = 20. The nonascending vector was computed by the method described in the 647 648 paragraph below (12). Denoting by  $R_S$  the infinite sequence of points in  $\Omega$  that is produced 649 by the superiorized version of the algorithm  $\mathbf{R}$  when applied to the problem S, we chose as our reconstruction  $x^* = O(S, 0.33, R_S)$ . For such a reconstruction we have, by the definition 650 of O, that  $Res_{S}(\boldsymbol{x}^{*}) \leq 0.33$ ; in other words, the output of the superiorization algorithm is 651 at least as constraints-compatible with S as the output of ASD-POCS. From the point of 652 view of TV-minimization, our  $\boldsymbol{x}^*$  is slightly better:  $TV(\boldsymbol{x}^*) = 826$ . 653

654 The superiorization reconstruction is displayed in figure 2(b). Visually it is similar to the 655 reconstruction produced by ASD-POCS. From the optimization point of view it achieves the 656 desired aim better than ASD-POCS does, since it results in smaller values for both  $Res_S$  **657** and for TV, even though only slightly.

That the two reconstructions in figure 2 are very similar is not surprising because a 658 comparison of the pseudo-codes reveals that the ASD-POCS algorithm  $in^{42}$  is essentially a 659 special case of the Superiorized Version of Algorithm P, even though it has been derived 660 from rather different principles. To obtain the ASD-POCS algorithm from our methodology 661 described here, we would have to choose an Algebraic Reconstruction Technique (ART; 662 see Chapter 11 of<sup>55</sup>) as the algorithm that we are superiorizing. Such a superiorization of 663 ART was reported in the earliest paper on superiorization<sup>27</sup>. For the illustration in our 664 665 current paper we decided to superiorize the block-iterative algorithm  $\mathbf{R}$  defined by (3). This illustrates the generality of the superiorization approach: it is applicable not only to 666 a large class of constrained optimization problems, but also enables the use of any of a 667 large class of iterative algorithms designed to produce a constraints-compatible solutions. 668 A recent publication aimed at producing an exact TV-minimizing algorithm based on the 669 block-iterative approach is<sup>44</sup>. 670

## 671 D. Effects of variations in the reconstruction approach

The reconstruction in figure 2(a) produced by ASD-POCS definitely "looks better" than 672 a reconstruction in<sup>31</sup>, which was obtained using superiorization from similar data. Since, as 673 discussed in the last paragraph of the previous subsection, the ASD-POCS algorithm in<sup>42</sup> 674 can be obtained as a special case of superiorization, it must be that some of the choices made 675 676 in the details of the implementations are responsible for the visual differences. An analysis of the implementational details adopted by the two approaches revealed several differences. 677 678 After removing these differences, the superiorization approach produced the image in figure 679 2(b), which is very similar to the reconstruction produced by ASD-POCS. We now list the 680 implementational choices that were made for superiorization to make its performance match 681 that of the reported implementation of ASD-POCS.

682 One implementational difference is in the stopping-rule of the iterative algorithm; that 683 is, the choice of  $\varepsilon$  in determining the output  $O(S, \varepsilon, R_S)$ . Since the data are noisy, the 684 phantom itself does not match the data exactly. In previously reported implementations of 685 superiorization it was assumed that the iterative process should terminate when an image 686 is obtained that is approximately as constraints-compatible as the phantom; in the case of 687 the phantom and the projections data on which we report here the value of  $Res_S$  for the 688 phantom is approximately 0.91, which is larger than its value (0.33) for the reconstruction 689 produced by ASD-POCS. The output  $O(S, 0.91, R_S)$  is shown in figure 3(a). This is a wonderfully smooth reconstruction, its TV value is only 771. However this smoothness 690 691 comes at a price: we loose not only the ability to detect the large tumor, but we cannot even see anatomic features (such as the ventricular cavities) inside the brain. So it appears 692 that, in order to see medically-relevant features in the brain, over-fitting (in the sense of 693 694 producing a reconstruction from noisy data that is more constraints-compatible than the 695 phantom) is desirable.

In the implementations that produced previously reported reconstructions by superior-696 ization, the number N in the Superiorized Version of Algorithm  $\mathbf{P}$  was always chosen to 697 be 1. It is possible that this is the wrong choice, making only this change to what lead to 698 699 the reconstruction in figure 2(b) results in the reconstruction shown in figure 3(b). That image appears similar to the image in figure 2(b), but it has a higher TV value, namely 832, 700 which is still very slightly lower than that of the ASD-POCS reconstruction. The choice 701 N = 20 was based on the desire to maintain consistency with what has been practiced using 702 ASD-POCS, see page 4790 of<sup>42</sup>. It appears that in the context of our paper the additional 703 704 computing cost due to choosing N to be 20 rather than 1 is not really justified. (We note that if d is selected using subgradients as discussed in the paragraph following (7) and thus 705 706 d is not guaranteed to be a nonascending vector for the TV function, then the choice of 707 20 rather than 1 for N results in a considerable improvement. However, an even greater improvement is achieved even with N = 1 by selecting d as recommended in this paper.) 708

709 Another important difference between the ASD-POCS implementation and the previous implementations of the superiorization approach is the size of the pixels in the reconstruc-710 tions. For the ASD-POCS reconstruction this was selected to be 0.376 mm by 0.376 mm. 711 In previously reported reconstructions by superiorization it was assumed that the edge of 712 a pixel should be the same as the distance between the parallel lines along which the data 713 are collected; that is, 0.752 mm for our problem S. This assumption proved to be false. 714 TV-minimization takes care of undesirable artifacts that may otherwise arise due to the 715 smaller pixels and this leads to a visual improvement. A superiorizing reconstruction with 716 the larger pixels, using  $\varepsilon = 0.33$  and N = 20, is shown in figure 3(c). (We note that the use 717 of smaller pixels during iterative x-ray CT reconstructions was also suggested in<sup>59</sup>. How-718



Figure 3: Reconstructions produced by varying some of the parameters in the algorithm that produced figure 2(b). (a) Changing the termination criterion form  $\varepsilon = 0.33$  to  $\varepsilon = 0.91$ . (b) Changing the value of N from 20 to 1. (c) Reconstructing with pixel size 0.752 mm by 0.752 mm instead of 0.376 mm by 0.376 mm. (d) Reconstructing with all the three changes of (a)-(c).

719 ever, that approach is quite different from what is presented here: its final result uses larger 720 pixels whose values are obtained by averaging assemblies of values provided by the iterative 721 process to the smaller pixels. There is no such downsampling in our approach, our final 722 result is presented using the smaller pixels. Its smoothness is due to reduction of TV by the 723 superiorization approach rather than to averaging pixel values in a denser digitization.)

Combining the use of the larger pixels with  $\varepsilon = 0.91$  and N = 1 results in the reconstruc-724 tion shown in figure 3(d). This reconstruction, for which the superiorization options were 725 726 selected according to what was done  $in^{31}$ , is visually inferior to those shown in our figure 2. The reconstructions displayed in figure 3 also illustrate another important point, namely 727 that even though the mathematical results discussed in this paper are valid for a large range 728 of choices of the parameters in the superiorization algorithms, for medical efficacy of the 729 reconstructions attention has to be paid to these choices since they can have a drastic effect 730 731 on the quality of the reconstruction.

It has been mentioned in Subsection IIB that except for the presence of  $\mathbf{Q}$  in (3), which 732 enforces nonnegativity of the components, **R** is identical to the algorithm used and illustrated 733  $in^{31}$ . It is known that CT reconstruction of the brain from many views does not suffer 734 from ignoring the fact that the components of the  $\boldsymbol{x}$ , which represent linear attenuation 735 coefficients, should be nonnegative; as is illustrated in figure 1(b). This remains so when 736 737 reconstructing from a few views using the method and data that we have been discussing: 738 if we do everything in exactly the same way as was done to obtain the reconstruction with TV value 826 that is shown in our figure 2(b) but remove Q from (3), then we obtain a 739 740 reconstruction in figure 4(a) whose TV value is 829.

Another variation that deserves discussion, because it has been suggested in the 741 literature<sup>22</sup>, is one that does not come about by making choices for the general approach of 742 743 the Superiorized Version of Algorithm **P** but rather by changing the nature of the approach. The variation in question is not applicable in general, but can be applied to the special 744 case when the algorithm to be superiorized is the  $\mathbf{R}$  defined by (3). It was suggested as 745 an improvement to the approach presented above with the choice N = 1. The idea was 746 based on recognizing the block-iterative nature of the algorithmic operator  $\mathbf{R}_{S}$  in (3) and 747 intermingling the perturbation steps of lines (vii)-(xvii) of the Superiorized Version of Al-748 749 gorithm **R** with the projection steps  $\mathbf{B}_{S_1}, \ldots, \mathbf{B}_{S_W}$  of (3). It was reported in<sup>22</sup> that doing this is advantageous to using the Superiorized Version of Algorithm  $\mathbf{R}$ . However, when we 750



Figure 4: Reconstructions by variations that do not fit into the framework within which the previously shown reconstructions were produced. (a) Not using nonnegativity in the algorithm. (b) Interleaving perturbations with blocks.

applied the variation of the Superiorized Version of Algorithm  $\mathbf{R}$  that is proposed in<sup>22</sup> to 751 the problem S that we have been using in this section, we ended up with the reconstruction 752 in figure 4(b) whose TV value is 920. This is not as good as what was obtained using the 753 version of the algorithm that produced the reconstruction in figure 2(b). We conclude that 754 the variation suggested  $by^{22}$ , which does not fit into the theory of our paper, does not have 755 an advantage over what we are proposing here, at least for the problem S that we have 756 been discussing in this section. We conjecture that the improvement reported  $in^{22}$  is due to 757 758 selecting d using subgradients as discussed in the paragraph following (7) and, as discussed earlier, such an improvement is not obtained if d is selected by the more appropriate method 759 760 recommended in this paper.

# 761 IV. DISCUSSION AND CONCLUSIONS

762 Constrained optimization is an often-used tool in medical physics. The methodology of763 superiorization is a heuristic (as opposed to exact) approach to constrained optimization.

764 Although the idea of superiorization was introduced in 2007 and its practical use has been demonstrated in several publications since, this paper is the first to provide a solid math-765 766 ematical foundation to superiorization as applied to the noisy problems of the real world. These foundations include a precise definition of constraints-compatibility, the concept of a 767 strongly perturbation resilient algorithm, simple conditions that ensure that an algorithm 768 is strongly perturbation resilient, the superiorized version of an algorithm and the showing 769 that the superiorized version of a strongly perturbation resilient algorithm produces outputs 770 771 that are essentially as constraints-compatible as those produced by the original version but are likely to have a smaller value of the chosen optimization criterion. 772

The approach is very general. For any iterative algorithm **P** and for any optimization criterion  $\phi$  for which we know how to produce nonascending vectors, the pseudocode given in Subsection II E automatically provides the version of **P** that is superiorized for  $\phi$ .

We demonstrated superiorization for tomography when total variation is used as the optimization criterion. In particular, we illustrated on a particular tomography problem that, in spite of its generality, superiorization produced a reconstruction that is as good as (from the points of view of constraints-compatibility and TV-minimization) what was obtained by the ASD-POCS algorithm that was specially designed for TV-minimization in tomography.

782

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#### Appendix

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## Conditions for strong perturbation resilience

**792** Theorem 1. Let **P** be an algorithm for a problem structure  $\langle \mathbb{T}, \mathcal{P}r \rangle$  such that, for all **793**  $T \in \mathbb{T}$ , **P** is boundedly convergent for  $T, \mathcal{P}r_T : \Omega \to \mathbb{R}$  is uniformly continuous and **794**  $\mathbf{P}_T : \Delta \to \Omega$  is nonexpansive. Then **P** is strongly perturbation resilient.

**795** *Proof.* We first show that there exists an  $\varepsilon \in \mathbb{R}_+$  such that  $O\left(T, \varepsilon, \left((\mathbf{P}_T)^k \boldsymbol{x}\right)_{k=0}^{\infty}\right)$  **796** is defined for every  $\boldsymbol{x} \in \Omega$ . Under the assumptions of the theorem, let  $\gamma \in \mathbb{R}_+$  be such **797** that  $\mathcal{P}r_T(\boldsymbol{y}(\boldsymbol{x})) \leq \gamma$ , for every  $\boldsymbol{x} \in \Omega$ . We prove that  $O\left(T, 2\gamma, \left((\mathbf{P}_T)^k \boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined **798** for every  $\boldsymbol{x} \in \Omega$  as follows. Select a particular  $\boldsymbol{x} \in \Omega$ . By uniform continuity of  $\mathcal{P}r_T$ , **799** there exists a  $\delta > 0$ , such that  $|\mathcal{P}r_T(\boldsymbol{z}) - \mathcal{P}r_T(\boldsymbol{y}(\boldsymbol{x}))| \leq \gamma$ , for any  $\boldsymbol{z} \in \Omega$  for which **800**  $||\boldsymbol{z} - \boldsymbol{y}(\boldsymbol{x})|| \leq \delta$ . Since **P** is convergent for *T*, there exists a nonnegative integer *K*, such **801** that  $\left\| (\mathbf{P}_T)^K \boldsymbol{x} - \boldsymbol{y}(\boldsymbol{x}) \right\| \leq \delta$ . It follows that

$$\left| \mathcal{P}r_{T}\left( \left( \mathbf{P}_{T} \right)^{K} \boldsymbol{x} \right) \right| \leq \left| \mathcal{P}r_{T}\left( \left( \mathbf{P}_{T} \right)^{K} \boldsymbol{x} \right) - \mathcal{P}r_{T}\left( \boldsymbol{y}\left( \boldsymbol{x} \right) \right) \right| + \left| \mathcal{P}r_{T}\left( \boldsymbol{y}\left( \boldsymbol{x} \right) \right) \right|$$

$$\leq 2\gamma.$$
(13)

802 Now let  $T \in \mathbb{T}$  and  $\varepsilon \in \mathbb{R}_+$  be such that  $O\left(T, \varepsilon, \left((\mathbf{P}_T)^k \boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined for every 803  $\boldsymbol{x} \in \Omega$ . To prove the theorem, we need to show that  $O\left(T, \varepsilon', R\right)$  is defined for every  $\varepsilon' > \varepsilon$ 804 and for every sequence  $R = (\boldsymbol{x}^k)_{k=0}^{\infty}$  of points in  $\Omega$  for which, for all  $k \ge 0$ , (6) is satisfied for 805 bounded perturbations  $\beta_k \boldsymbol{v}^k$ . Let  $\varepsilon'$  and R satisfy the conditions of the previous sentence.

For  $k \geq 0$ , we have, due to the nonexpansiveness of  $\mathbf{P}_T$ , that

$$\left\|\boldsymbol{x}^{k+1} - \mathbf{P}_T \boldsymbol{x}^k\right\| = \left\|\mathbf{P}_T \left(\boldsymbol{x}^k + \beta_k \boldsymbol{v}^k\right) - \mathbf{P}_T \boldsymbol{x}^k\right\| \le \left\|\beta_k \boldsymbol{v}^k\right\|.$$
(14)

**806** Denote  $\|\beta_k \boldsymbol{v}^k\|$  by  $r_k$ . Clearly,  $r_k \in \mathbb{R}_+$  and it follows from the definition of bounded **807** perturbations that  $\sum_{k=0}^{\infty} r_k < \infty$ .

808 We next prove by induction that, for every pair of nonnegative integers k and i,

$$\left\|\boldsymbol{x}^{k+i} - \left(\mathbf{P}_{T}\right)^{i} \boldsymbol{x}^{k}\right\| \leq \sum_{j=k}^{k+i-1} r_{j}.$$
(15)

**809** Let k be an arbitrary nonnegative integer. If i = 0, then the value is zero on both sides of **810** the inequality and hence (15) holds. Now assume that (15) holds for an integer  $i \ge 0$ . Then, **811** by (14) and the nonexpansiveness of  $\mathbf{P}_T$ ,

$$\begin{aligned} \left\| \boldsymbol{x}^{k+i+1} - (\mathbf{P}_T)^{i+1} \, \boldsymbol{x}^k \right\| &\leq \left\| \boldsymbol{x}^{k+i+1} - \mathbf{P}_T \boldsymbol{x}^{k+i} \right\| \\ &+ \left\| \mathbf{P}_T \boldsymbol{x}^{k+i} - (\mathbf{P}_T)^{i+1} \, \boldsymbol{x}^k \right\| \\ &\leq r_{k+i} + \left\| \boldsymbol{x}^{k+i} - (\mathbf{P}_T)^i \, \boldsymbol{x}^k \right\| \\ &\leq r_{k+i} + \sum_{j=k}^{k+i-1} r_j \\ &= \sum_{j=k}^{k+i} r_j, \end{aligned}$$
(16)

812 which completes our inductive proof. A consequence of (15) is that, for every pair of non-813 negative integers k and i,

$$\left\|\boldsymbol{x}^{k+i} - \left(\mathbf{P}_T\right)^i \boldsymbol{x}^k\right\| \le \sum_{j=k}^{\infty} r_j.$$
(17)

814 Due to the summability of the nonnegative sequence  $(r_k)_{k=0}^{\infty}$ , the right-hand side (and hence 815 the left-hand side) of this inequality gets arbitrarily close to zero as k increases.

816 Since  $\mathcal{P}r_T$  is uniformly continuous, there exists a  $\delta$  such that, for all  $\boldsymbol{x}, \boldsymbol{y} \in \Omega$ , 817  $|\mathcal{P}r_T(\boldsymbol{x}) - \mathcal{P}r_T(\boldsymbol{y})| \leq \varepsilon' - \varepsilon$  provided that  $||\boldsymbol{x} - \boldsymbol{y}|| \leq \delta$ . Select a k so that  $\sum_{j=k}^{\infty} r_j \leq \delta$ . 818 By the assumption that  $O\left(T, \varepsilon, \left((\mathbf{P}_T)^k \boldsymbol{x}\right)_{k=0}^{\infty}\right)$  is defined for every  $\boldsymbol{x} \in \Omega$ , there exists a 819 nonnegative integer i for which  $\mathcal{P}r\left((\mathbf{P}_T)^i \boldsymbol{x}^k\right) \leq \varepsilon$ . From (17) we have, for this k and i, 820 that  $||\boldsymbol{x}^{k+i} - (\mathbf{P}_T)^i \boldsymbol{x}^k|| \leq \delta$  and, hence,

$$\begin{aligned} \left| \mathcal{P}r_{T}(\boldsymbol{x}^{k+i}) \right| &\leq \left| \mathcal{P}r_{T}(\boldsymbol{x}^{k+i}) - \mathcal{P}r_{T}\left( \left( \mathbf{P}_{T} \right)^{i} \boldsymbol{x}^{k} \right) \right| \\ &+ \left| \mathcal{P}r_{T}\left( \left( \mathbf{P}_{T} \right)^{i} \boldsymbol{x}^{k} \right) \right| \\ &\leq (\varepsilon' - \varepsilon) + \varepsilon = \varepsilon', \end{aligned}$$
(18)

**821** proving that  $O(T, \varepsilon', R)$  is defined.  $\Box$ 

822

## Nonascending vectors for convex functions

823 Theorem 2. Let  $\phi : \mathbb{R}^J \to \mathbb{R}$  be a convex function and let  $\boldsymbol{x} \in \mathbb{R}^J$ . Let  $\boldsymbol{g} \in \mathbb{R}^J$  satisfy the 824 property: For  $1 \le j \le J$ , if the *j*th component  $g_j$  of  $\boldsymbol{g}$  is not zero, then the partial derivative 825  $\frac{\partial \phi}{\partial x_j}(\boldsymbol{x})$  of  $\phi$  at  $\boldsymbol{x}$  exists and its value is  $g_j$ . Define  $\boldsymbol{d}$  to be the zero vector if  $\|\boldsymbol{g}\| = 0$  and to 826 be  $-\boldsymbol{g}/\|\boldsymbol{g}\|$  otherwise. Then  $\boldsymbol{d}$  is a nonascending vector for  $\phi$  at  $\boldsymbol{x}$ . For  $1 \le j \le J$ , let  $s_j$  be  $g_j/|g_j|$  for  $j \in I$  and be 0 otherwise, and let  $e^j \in \mathbb{R}^J$  be the vector all of whose components are zero except for the *j*th, which is one. Then, for  $1 \le j \le J$ , there exists a  $\delta_j > 0$  such that, for  $0 \le \lambda_j \le \delta_j$ ,

$$\phi\left(\boldsymbol{x} - \lambda_j s_j \boldsymbol{e}^j\right) \le \phi\left(\boldsymbol{x}\right). \tag{19}$$

832 This is obvious if  $s_j = 0$ . Otherwise,  $\frac{\partial \phi}{\partial x_j}(\boldsymbol{x})$  exists and indicates  $\phi$  increases at  $\boldsymbol{x}$  if  $s_j = 1$ 833 or that  $\phi$  decreases at  $\boldsymbol{x}$  if  $s_j = -1$ . The existence of the desired  $\delta_j$  can be derived from the 834 standard definition of the partial derivative as a limit.

835 We define  $\delta > 0$  by

$$\delta = \frac{\|\boldsymbol{g}\|}{J} \min_{j \in I} \left\{ \frac{\delta_j}{|g_j|} \right\}.$$
(20)

**836** Then we have that, for  $0 \le \lambda \le \delta$ ,

$$\phi \left( \boldsymbol{x} + \lambda \boldsymbol{d} \right) = \phi \left( \boldsymbol{x} - \lambda \sum_{j=1}^{J} \frac{|g_j|}{\|\boldsymbol{g}\|} s_j \boldsymbol{e}^j \right)$$

$$= \phi \left( \sum_{j=1}^{J} \frac{1}{J} \left( \boldsymbol{x} - \lambda J \frac{|g_j|}{\|\boldsymbol{g}\|} s_j \boldsymbol{e}^j \right) \right)$$

$$\leq \frac{1}{J} \sum_{j=1}^{J} \phi \left( \boldsymbol{x} - \lambda J \frac{|g_j|}{\|\boldsymbol{g}\|} s_j \boldsymbol{e}^j \right)$$

$$\leq \frac{1}{J} \sum_{j=1}^{J} \phi \left( \boldsymbol{x} \right)$$

$$= \phi \left( \boldsymbol{x} \right).$$
(21)

**837** The first inequality above follows from the convexity of  $\phi$  and the second one follows from **838** (19), with  $\lambda_j$  defined to be  $\lambda J \frac{|g_j|}{||g||}$ , combined with (20). Thus d is a nonascending vector for **839**  $\phi$  at  $\boldsymbol{x}$ .  $\Box$ 

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<sup>840 \*</sup> Author to whom correspondence should be addressed; Electronic address: gaborther841 man@yahoo.com; URL: http://www.dig.cs.gc.cuny.edu/~gabor/index.html

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