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Vorwort

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In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe sollen sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen werden.

Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Dieter Prätzel-Wolters

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

Trade-off bounds and their effect in multi-criteria IMRT planning

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Abstract. One approach to multi-criteria IMRT planning is to automatically calculate a data set of Pareto-optimal plans for a given planning problem in a first phase, and then interactively explore the solution space and decide for the clinically best treatment plan in a second phase. The challenge of computing the plan data set is to assure that all clinically meaningful plans are covered and that as many as possible clinically irrelevant plans are excluded to keep computation times within reasonable limits. In this work, we focus on the approximation of the clinically relevant part of the Pareto surface, the process that consititutes the first phase.

It is possible that two plans on the Parteto surface have a very small, clinically insignificant difference in one criterion and a significant difference in one other criterion. For such cases, only the plan that is clinically clearly superior should be included into the data set. To achieve this during the Pareto surface approximation, we propose to introduce bounds that restrict the relative quality between plans, so called trade-off bounds. We show how to integrate these trade-off bounds into the approximation scheme and study their effects.

The proposed scheme is applied to two artificial cases and one clinical case of a paraspinal tumor. For all cases, the quality of the Pareto surface approximation is measured with respect to the number of computed plans, and the range of values occurring in the approximation for the different criteria is compared. Through enforcing trade-off bounds, the scheme focuses the approximation to the subset of Pareto-optimal plans that are clinically relevant, resulting in a better approximation quality achieved with significantly fewer plans. Thus, trade-off bounds are an effective tool to focus the planning and to reduce computation time.

AMS classification scheme numbers: 90C29, 90C25

1. Background and purpose

Multi-criteria IMRT planning is a planning paradigm that allows the planner to postpone the choice of a compromise between the different planning goals till the point where the chances and limitations of the case at hand are already explored.

To achieve that, the planning process is split into two phases ([Küfer *et al.*, 2000, Cotrutz *et al.*, 2001, Lahanas *et al.*, 2003, Küfer *et al.*, 2003]). The first phase is used to automatically explore the possible compromises and approximate the set of the Pareto-optimal plans. The second phase uses decision support tools to ease the selection of the final plan. Using such tools, all approximated planning options can be explored interactively ([Monz *et al.*, 2008]). A multi-criteria approach and adequate navigation tools lead to effective plan determination processes that involve less active planning time ([Thieke *et al.*, 2007]).

Because the set of plans used for decision making is determined during the first phase, it is clear that the quality of the final result is greatly influenced by phase one's scheme. Currently, the state-of-the-art are sandwiching schemes ([Solanki *et al.*, 1993, Klamroth *et al.*, 2002, Craft *et al.*, 2006]), which are driven iteratively by the quality of the resulting approximation.

Nevertheless, the approximation often contains plans that are not clinically meaningful. To exclude those plans absolute bounds on the different criteria are used. However, the choice of those bounds is difficult: if chosen too strict they might exclude good plans, but if chosen too permissive the approximation will spend effort calculating clinically meaningless plans.

Therefore, we propose to use rather permissive absolute bounds and in addition, bounds that restrict relative quality, so called trade-off bounds. We describe how to directly include them into the approximation scheme and study their effect for two artificial and one clinical case. Furthermore, we describe how the integration of the trade-off bounds removes boundary artefacts in the known approximation algorithms.

2. Material and methods

Multi-criteria optimization considers different measures of quality – called criteria – for a solution as separate entities. Consequently, the quality of a solution is recorded in a vector as opposed to a single number in standard optimization. Two arbitrary vectors might not be comparable, e.g. $\binom{2}{1}$ is neither greater nor smaller than $\binom{1}{2}$. Thus, an optimal solution cannot be identified and a new notion of optimality is needed.

A multi-criteria problem is denoted in the following way:

$$\text{v-}\min \left\{ \mathbf{f}(\mathbf{x}) \;\middle|\; \mathbf{x} \in \mathcal{X} \right\} \tag{1}$$

where v- min refers to vector-valued optimization.

The most common concept of optimality in multi-criteria optimization is Pareto-optimality. A feasible solution $\mathbf{x} \in \mathcal{X}$ is Pareto-optimal, if improving one criterion can only be achieved by degrading other criteria. This means that Pareto-optimal solutions are compromises that cannot be improved.

In this paper, we will almost exclusively work in the so called criterion or objective space. Here, each plan $\mathbf{x}$ is represented by the k-dimensional vector that stores each of its criteria values, i.e. a plan $\mathbf{x}$ is represented instead using its corresponding image $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^k$, where $\mathbf{f}$ is a vector of real valued function.

In IMRT planning, the optimization model is described using functions over radiation doses $\mathbf{d}(\mathbf{x})$ produced by a vector of non-negative beamlet intensities $\mathbf{x} \geq \mathbf{0}$. The other constraints that define the set $\mathcal{X}$ are given by convex functions $\mathbf{g}(\mathbf{x})$. Hence, problem (1) may be reformulated as following,

$$\text{v-}\min \left\{ \mathbf{f}(\mathbf{x}) \;\middle|\; \mathbf{f}(\mathbf{x}) \leq \mathbf{b}, \mathbf{g}(\mathbf{x}) \leq \mathbf{b}', \mathbf{x} \geq \mathbf{0} \right\}, \tag{2}$$

where $\mathbf{b}$ are upper bounds on the criteria functions.

We use convex functions of the dose as criteria in our models. Convexity is necessary in order to apply efficient deterministic optimization methods to the problems under consideration. Convex minimization techniques are able to provide optimality certificates. In contrast to the convex case, finding the global optimum for non-convex objective functions is usually not possible within a reasonable time and computational effort. In addition, the properties of the Pareto surface, which result from the convexity assumption, will be exploited in the approximation scheme.

Examples of convex functions which are commonly used in the context of IMRT planning and general (non-convex) functions that can be substituted by convex descriptions are given in [Romeijn *et al.*, 2004]. They setup framework contains TCP, NTCP and Niemierko's generalized EUD ([Niemierko, 1999]) among others. Furthermore, so-called tail EUDs [Bortfeld *et al.*, 2008] and deviations from a prescribed dose like standard deviatoion fall into the class of convex functions. In [Wu *et al.*, 2002] and [Wu *et al.*, 2005], generalized EUD objectives are shown to be able to tailor dose as wanted in IMRT planning. Combined with tail EUDs and deviations we are able to formulate expressive models. Taking into account the previously mentioned reasons, in this work, we only consider convex criteria.

In convex models, the criterion vectors of the Pareto-optimal plans form a coherent connected set, that is part of the surface of a convex body. This set $\left\{ \mathbf{f}(\mathbf{x}) \middle| \; \mathbf{x} \text{ is Pareto-optimal} \right\}$ is called Pareto surface.

Figure 1 visualizes the important effects of convexity for the approximation of the Pareto surface. First, by the definition of convexity, the true criteria values $\mathbf{f}(\tilde{\mathbf{x}})$ of a convex combination of plans – a mixed plan $\tilde{\mathbf{x}}$ – are better than the convex combination of the corresponding criterion value vectors:

$$\mathbf{f}(\tilde{\mathbf{x}}) = \mathbf{f}\Big(\sum_i \mathbf{t}_i \mathbf{x}^i\Big) \leq \sum_i \mathbf{t}_i \mathbf{f}(\mathbf{x}^i), \quad \sum_i \mathbf{t}_i = 1, \ \mathbf{t} \geq \mathbf{0}$$

Thus, any convex combination of plans fulfills the given upper bounds $\mathbf{b}$ and $\mathbf{b}'$. Since the intensities $\mathbf{x} \geq \mathbf{0}$ are feasible as well, any convex combination of plans is feasible. Moreover, the convex combination of criteria vectors is an upper bound for the performance of such a combination and can therefore be used as a pessimistic prediction of such a plan's quality.

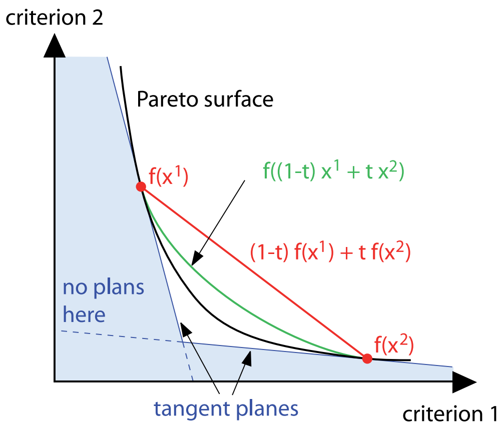


Figure 1. The outer curve is the Pareto surface. The dots are two computed plans. The straight line is given by the convex combinations of the two plans' criterion vectors: $(1-t)\mathbf{f}(\mathbf{x}^1) + t\mathbf{f}(\mathbf{x}^2)$. The inner curve is instead given by the criterion vectors of the convex combinations of the two plans: $\mathbf{f}\big((1-t)\mathbf{x}^1 + t\mathbf{x}^2\big)$. The area at the bottom is delimited by the two plans' tangent planes to the Pareto surface. The area is the part of the objective space that given the tangent planes is known to contain no plans.

Second, by a basic theorem of convex analysis (see e.g. [Rockafellar, 1970]) the tangent plane to a convex function at any point generally is a lower bound for the function. Therefore, no plan can have criterion values that lie below the tangent plane of any other calculated plan. This is used to exclude large parts of the criterion space from consideration.

Combining the two bounds, we can enclose the volume which contains the Pareto surface. The thickness of this volume sandwiching the Pareto surface provides a pessimistic estimation of the approximation error. Some of the known sandwiching methods measure the Euclidean distance ([Solanki *et al.*, 1993, Craft *et al.*, 2006]), some ([Klamroth *et al.*, 2002]) including our approach use the smallest stretching factor that makes the inner approximation contain the outer. Thus, a approximation quality of 1 would indicate that the inner and outer approximation are the same. For either way of measuring distance a facet of the inner and an extreme point of the outer approximation are detected that delimit the biggest distance in the sandwich.

After that an optimization problem is formulated that yields a new plan within that part of the sandwich. Thereby, a new point for the inner approximation and a tangent plane for the outer approximation is added, that significantly reduce the local size of the sandwich (see figure 3(b)). This way, the approximation quality is improved until either a specified quality threshold or a timeout is reached. Either way, an upper bound on the achieved approximation quality is known.

The known sandwiching methods all start with an initial set of k Pareto-optimal plans, each one minimizing one of the k components of $\mathbf{f}(\mathbf{x})$. The k points and their tangent planes are used to set up the first enclosing volume. After that, plans are added, where the sandwich is thickest. Unfortunately, this approach usually does not cover the boundary parts of the Pareto surface, which leads to artifacts in the algorithms that need specific treatment ([Solanki *et al.*, 1993, Craft *et al.*, 2006]) or even make the algorithm cycle ([Klamroth *et al.*, 2002]).

2.1. Trade-offs and ordering cones

The trade-off of two plans with respect to two of the criteria, i.e. a so-called partial trade-off ([Miettinen, 1999, Chankong and Haimes, 1983]) measures the change in one criterion relative to the second criterion. Very large or very small trade-offs – that become large when changing the roles of the criteria – indicate that a high price in one criterion has to be paid for a relatively small improvement in the other criterion.

Geometrically, this corresponds to very steep or very flat parts of the Pareto surface. We thus want to exclude the parts of the Pareto surface that are steeper of flatter than some pre-specified trade-off bound. The tool to accomplish this are ordering cones.

Ordering cones contain the subset of the criterion space that is dominated by the origin. The ordering cone corresponding to Pareto-optimality is the non-negative orthant. If a plan $\mathbf{x}^1$ is Pareto-optimal, there is no other plan $\mathbf{x}^2$, such that the non-negative orthant attached to $\mathbf{f}(\mathbf{x}^2)$ contains the original plan's criterion vector $\mathbf{f}(\mathbf{x}^1)$ (see figure 2(a)). Using the non-negative orthant, arbitrary slopes of the Pareto surface are admissible, i.e. 0 and arbitrarily big values.

If there is a certain maximum trade-off that a planner is willing to tolerate – say a gain of 1 unit in one criterion for a loss of 5 units in a second criterion – one can define a ray representing the corresponding slope. Adding the new ray to the orthant's bounding rays yields a somewhat larger cone (details see [Monz, 2006]). This larger cone marks plans with poor trade-off as being dominated. Including the this more general

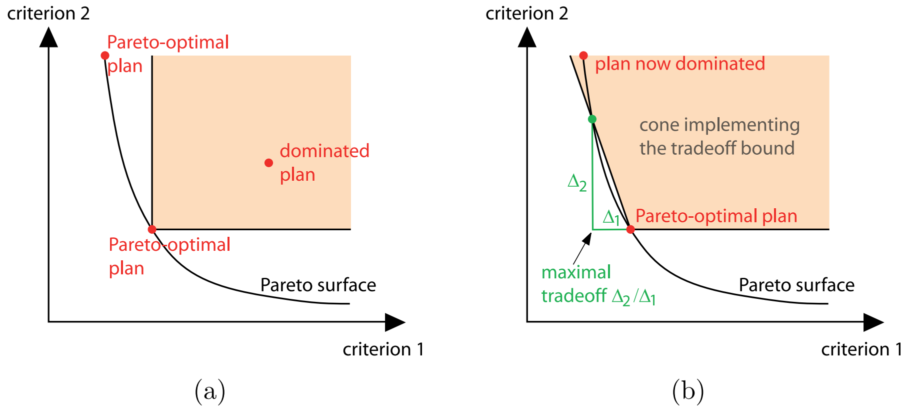


Figure 2. A Pareto-optimal plan dominates an area defined using a so called ordering cone, larger regions are discarded using a broader ordering cone than the non-negative orthant. The trade-off between two non-dominated plans is represented as a geometric property of the vector difference between these plans, an enlarged ordering cone can discard vectors with an unsatisfactory trade-off ratio.

notion of optimality into the approximation ensures that no plans with bad trade-offs are considered.

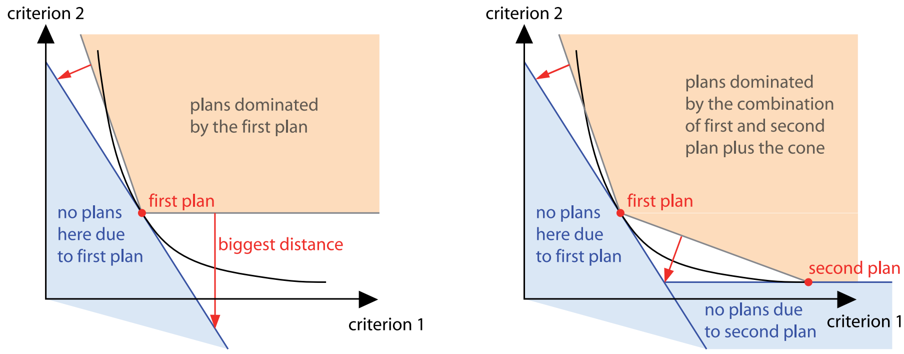
2.2. Including trade-offs into the approximation

Given a set of maximally tolerable trade-offs and thereby a corresponding ordering cone, we propose to use a sandwiching procedure to approximate the Pareto surface *plus* the ordering cone, i.e. the union of the ordering cone attached to each point of the Pareto surface.

Furthermore, we add the ordering cone to the inner approximation as well. The latter has the interpretation of "any plan of the approximation also represents all points that it dominates".

These seemingly small changes have a surprisingly big effect. Now, having calculated a first plan, our inner approximation is already a set – the plan plus the ordering cone – and can therefore be used to sandwich the Pareto surface. Thus, we are freed from calculating a set of k plans to start the approximation scheme.

Adding a cone to the Pareto surface and the approximation ensures that we have a sensible notion of the distance between the surface and the approximation even in parts that are not yet approximated with plans. For this reason, we get rid of the problems and special cases that the known sandwiching methods have at the boundary of their approximation. So, even adding the non-negative orthant, i.e. using our scheme with no trade-off bounds, has a positive effect on the algorithm in terms of achieved quality and globally meaningful distance estimation.



(a) (b)

Figure 3. The first computed plan sets a initial inner approximation, in which all plans dominated by the first plan are included. The tangent plane of the first plan forms the initial outer approximation. The biggest distance between both approximations is identified and a second plan is generated in this area to decrease the approximation error as much as possible. The inner approximation is now composed of the convex combination of the two plans plus the ordering cone. The outer approximation is given by the two tangent planes.

Finally, the proposed approximation scheme only approximates the optimal set with respect to the ordering cone, i.e. the subset of Pareto-optimal plans that fulfills the trade-off bounds. This focuses the calculation to the relevant bits, thereby decreasing running times to reach a given quality threshold or obtaining a better quality for the same number of plans.

3. Results and discussion

We apply the approximation scheme to two artificial cases and a clinical case to study the effects of adding trade-off bounds. The two artificial cases feature two and three criteria and therefore the approximation obtained for different ordering cones can be easily visualized and understood. The clinical case demonstrates that the effects transfer to realistic examples. We compare the approximation quality achieved over the number of plans for the different considered cones. Furthermore, DVHs from plans lying at the boundaries of the different approximations are shown.

In both artificial cases we set up the approximation using a *small*, *medium* and a *large cone* and simple optimization models. In the small cone an improvement of one unit in any criterion is allowed even if other criteria worsen by 1000 units. The trade-off is practically not bounded and, thus, the *small cone* considers virtually all Pareto-optimal points.

Real trade-off bounds are used to define the medium and large cone. For the medium cone, an improvement of one unit in any criteria is accepted only if it does not worsen any

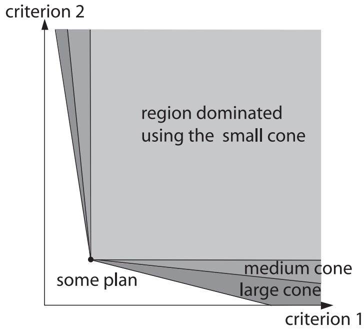


Figure 4. The small, medium and large cone for a two criteria case. The boundary rays of the small cone are almost parallel to the axes with trade-offs of 1:1000 and 1000:1. Thus, virtually all Pareto-optimal plans are non-dominated for this cone. The medium cone enlarges the area considered as dominated compared to the small cone (1:10, 10:1). The large cone defines an even greater area as being dominated. It is non-symmetric due to different trade-off bounds for the trade-off for tumor improvement and the improvement of the organ at risk. Thus, the ray pointing to the top is steeper (1 : 6.7) than the ray to the right is flat (4:1).

other criterion by more than 10 units. The large cone specifies trade-off bounds of 1 to 4 between an organ at risk and either an organ at risk or a tumor criterion. For improving the tumor a bound of 1 to 6.7 is accepted (see Figure 5). Thus, tumor improvements may have a higher price than improvements in organs at risk. In the clinical case, a more elaborated optimization model is used and two cones are considered: the small and the medium cone.

3.1. Horseshoe target

The first case that we are going to consider is a horse shoe target case – a two-dimensional abstraction of a paraspinal case (see Figure).

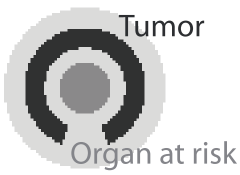


Figure 5. The tumor area almost completely surrounds the organ risk in the center.

For this case we set up a model consisting of two criteria and two constraints. The two criteria are a standard deviation from the desired value of 66 Gy for the tumor and an EUD for the organ at risk. The two criteria are bounded by values of 15 and 60 respectively. We have chosen loose absolute bounds for the criteria, in order to better demonstrate the effect of the trade-off bounds.

The number of points required to achieve a certain quality will normally show an

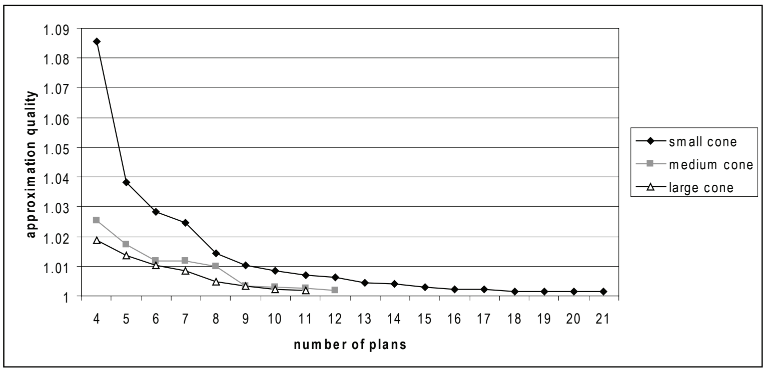
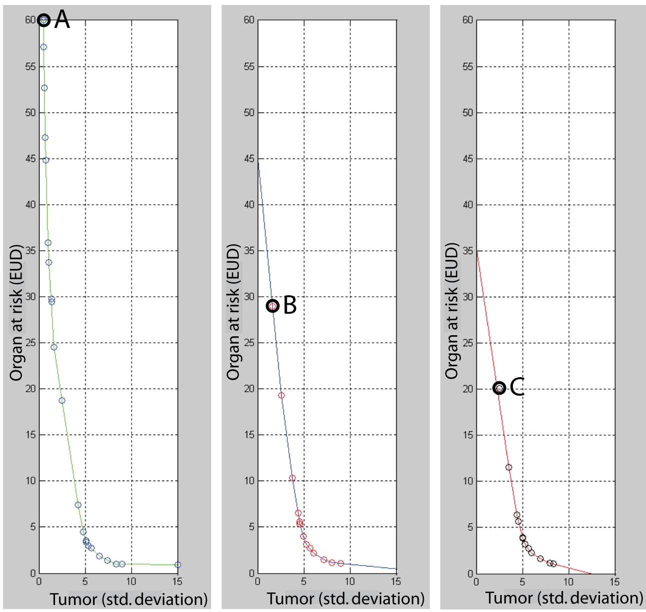


Figure 6. Quality achieved over the number of plans for the different cones in the horseshoe target case. The graph does not start with the first plan to reduce the necessary y-axis range.

exponential decline, due to the exponential behavior of the number of facets considered in the approximation – a fact that can be seen in the shown graphs. Due to that behaviour a lot more points are needed for the small cone to reach the quality for the small and medium cone. This effect would even be more pronounced, if the aspired quality level would have been closer to 1.

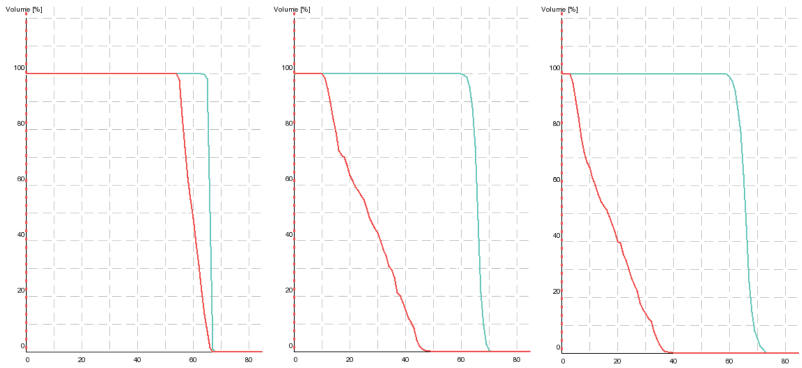


(a) Small cone (b) Medium cone (c) Large cone

Figure 7. The approximations to the horseshoe target's two dimensional Pareto surface for the different cones. The best possible tumor plan is marked in all three graphs. The line continuing from there is the boundary ray of the ordering cone.

Figure 7 visualizes the different approximations of the Pareto surface for the different cones. The approximations obtained with increasingly thougher trade-off bounds demonstrate how the steep and flat parts of the Pareto surface are discarded.

For all three cones the most interesting area in terms of trade-off quality is approximated adequately using roughly the same number of points. But for the small case 9 additional points are included into the approximation that yield small improvements in the tumor but significantly worse plan quality in the organ at risk.



(a) Plan A (b) Plan B (c) Plan C

Figure 8. DVH-Plots for the preselected plans. One can see that there is a dramatic improvement for the organ at risk for a very small price in terms of tumor quality.

The DVH-Plots for the plans marked as A, B and C are presented in Figure 8. In these pictures the trade-off can be easily compared. Although plan A in Figure 7 is an Pareto-optimal plan, plans with better "balance" can be found further away from the Pareto surface's boundary, as shown in subfigures 8(b) and 8(c).

3.2. Prostate Phantom

The second artificial case that we consider is a two-dimensional abstraction of a prostate case. Here, the target structure in the center is surrounded by two organs at risk, which represent the bladder and rectum (see Figure 9).

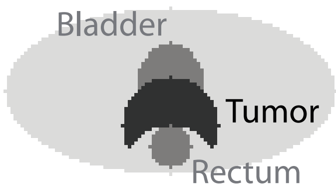


Figure 9. An artificial two dimensional case, where the target is surrounded by two risk structures. An abstraction of a prostate case.

We use standard deviation in the target and EUD functions in both organs at risk as criteria. We restrict the standard deviation to be less than 5, and the EUD functions to be less than 70. Again, we have chosen loose EUD bounds, in order to demonstrate how the trade-off deteriorates close to the Pareto surface boundary.

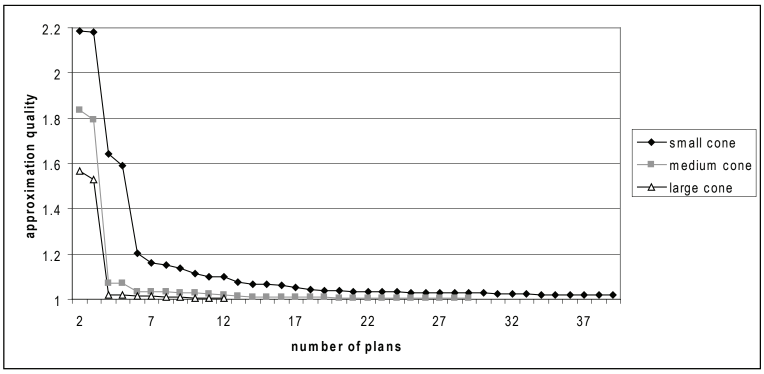


Figure 10. Quality achieved over the number of plans for the different cones in the prostate phantom case.

The graphs show that a noticable extra number of plans is needed to achieve a comparable quality for the smaller cones. Due to the higher dimension of the case the effect is even more pronounced than in the two dimensional case.

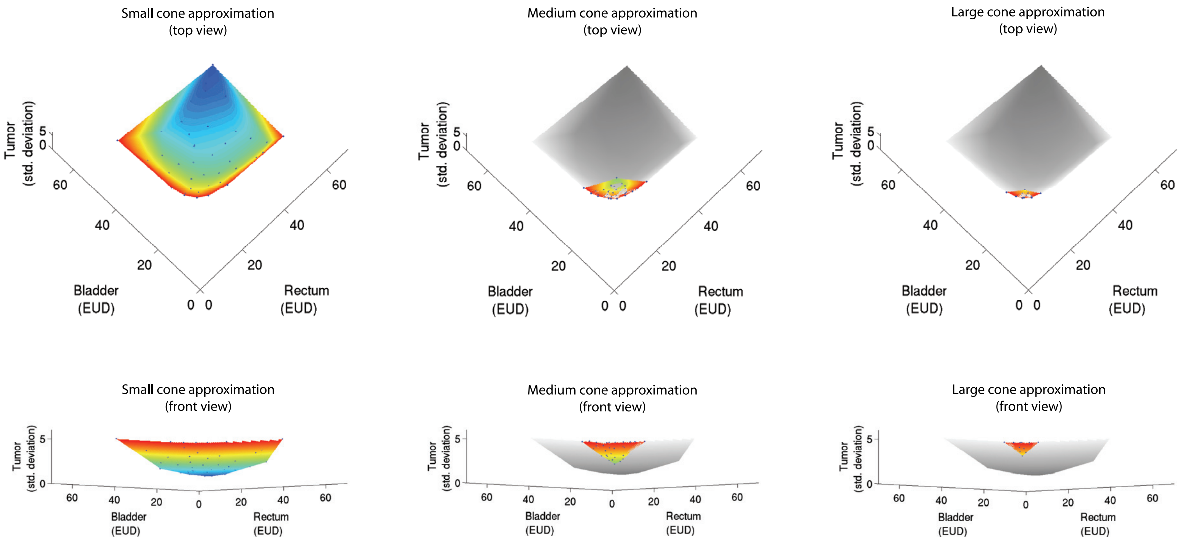
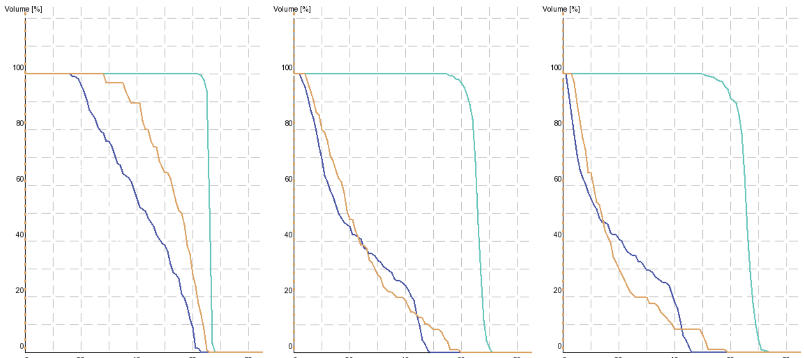


Figure 11. Prostate phantom Pareto surface approximations using different cones. The approximations are shown from the top and from the front. The small dots are the plans that make up the approximation. The grey area depicts the small cone approximation. One can see the dramatic reduction of the considered area, when the trade-off bounds get stronger.

Figure 11 is a plot of the Pareto surface approximation for the different cones. It nicely demonstrates how the use of trade-off bounds focusses the approximation to the interesting part of the Pareto surface. In particular, the change from the smalll to the medium cone reduces the area approximation drastically.

In Figure 12, we present DVH-Plots of the best tumor plan for each approximation.

Note that relatively small improvements of the tumor produce a dramatically worse EUDs for the organs at risk.



(a) Small cone (b) Medium cone (c) Large cone

Figure 12. DVH-Plots of the best tumor plan contained in the approximation for the different cones in the Prostate Phantom artificial case.

Some may consider the best tumor plan in the medium cone case to be better than the corresponding plan in the large cone case. For those people the trade-off bounds incorporated in the large cone are chosen too strict. Nevertheless, the case demonstrates the effectiveness of trade-off bounds as a tool to focus the attention to the interesting part of the Pareto surface, even if the actual choice of the trade-off bounds needs further investigation.

3.3. Paraspinal case

In this clinical case, shown in Figure 13, a tumor surrounds the spinal cord and the cauda. Kidneys and bowel are also considered as risk structures in the planning setup.

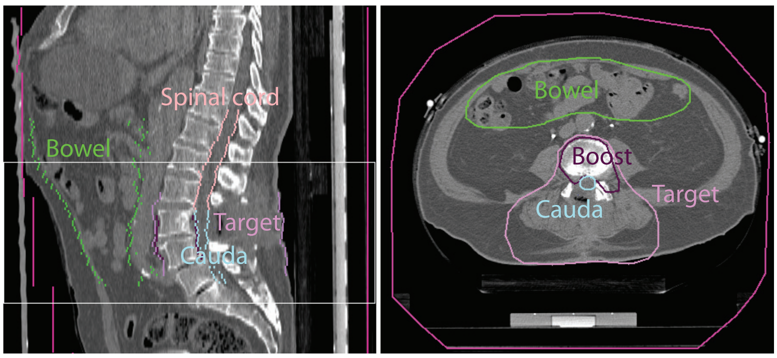


Figure 13. Tumor surrounding the lower part of the spinal cord and parts of the cauda. The tumor is divided into a target and a boost area for the planning. The kidneys and the bowel are considered as further organs at risk.

We use a standard deviation for the target and the boost volume with reference values of 51 Gy and 60 Gy respecively and restrict the deviations by 5 and 7. To further improve the tumor irradiation we introduce tail EUDs to restrict the under dose to the target and the boost. We use the same reference values and bounds of 3.7 and 2.5 respectively.

For the spinal cord, the cauda and the bowel risk structures we use EUDs and constrain each of them by 70. The kidneys are just considered using constraints. We restrict the mean doses by 6.5.

For this case only the approximations for the small and the medium cone are considered. Figure 14 presents the quality of the computed approximation over the number of plans. Here, not even four times the number of plans suffices to reach the same approximation quality.

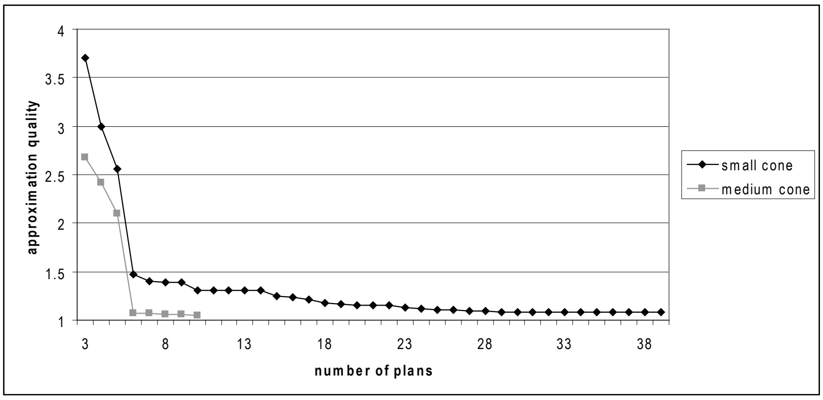
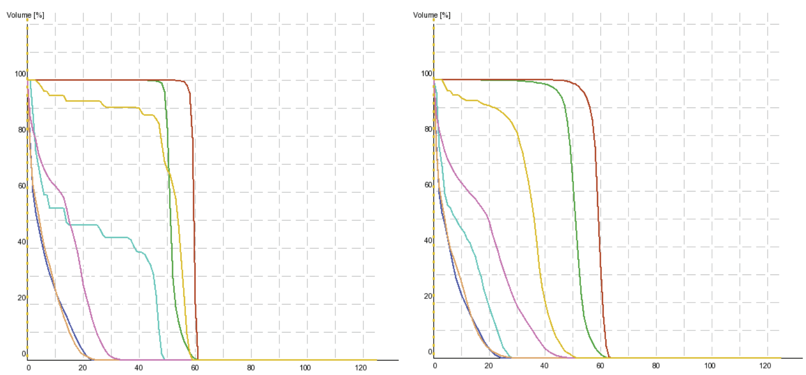


Figure 14. Quality achieved over the number of plans in the paraspinal case for the small and medium cone.

As stringent constraints are enforced in tumor structures, the resulting Pareto surface tends to kink in areas which consequently provide poor trade-offs. Being able to discard such areas algorithmically contributes greatly to reduce the approximation running time.



(a) Small cone (b) Medium cone

Figure 15. DVH-Plots of the plans with the best target value fixed and the best possible boost value attainable under that restriction for the two approximations.

The two plans that we have chosen to demonstrate the effects of the trade-off bounds are the plans with the best target value and the best possible boost value attainable with the target value being fixed (see Figure 15). In particular, the cauda and spinal cord curves - the two curves with the stair shaped middle part - are dramatically improved, while the target and boost curves suffer with regard to their under dose. Again, one could argue that the trade-off bounds were chosen too strict. Still, we want to focus here on demonstrating that trade-offs are an effective tool, rather than proposing trade-off bounds for specific clinical cases.

4. Conclusions

The Pareto surface obtained from convex IMRT problems can be represented using a convex combination of Pareto-optimal plans. Each such plan is supported by a tangent plane. The combination of the inner approximation provided by the convex combination of plans and the outer approximation given by the tangent planes can be used to estimate the approximation quality and to thereby steer the approximation scheme.

However, the approximation of the whole Pareto surface usually contains a large portion of plans with poor trade-off. By enforcing trade-off bounds those plans can be excluded from consideration. Trade-off bounds can be integrated into the approximation scheme by adding an ordering cone incorporating the trade-off bounds to the inner approximation. Besides the restriction of trade-offs the approximation scheme thereby gets rid of boundary artefacts present in all known sandwiching schemes. It is therefore advisable to add the ordering cone even when no trade-off bounds are considered.

Numerical results in two artificial and one clinical case show that trade-off bounds are an effective tool to discard uninteresting regions, thus drastically decreasing the computation time needed for the approximation. Moreover, they focus the attention to the interesting area and thus have the potential to also speed up the plan selection process.

Although, trade-off bounds have shown to be an effective tool it is not yet clear how to sensibly choose the specific bounds. Here, future planning studies for the respective treatment sites are needed.

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