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Mixed-Integer Nonlinear Design Optimization of a Superconductive Magnet with Surrogate Functions

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***Abstract*—The numerical optimization of continuous parameters in electrotechnical design using electromagnetic field simulation is already standard. When integer-valued variables are involved, the complexity of the optimization problem rises drastically. In this paper, we describe a new sequential surrogate optimization approach for simulation-based mixed-integer nonlinear programming problems. We apply the method for the optimization of combined integer- and real-valued geometrical parameters of the coils of a superconductive magnet.**

I. Introduction

Besides random search and sampling methods, surrogate optimization techniques have been found to be powerful for overcoming the specific difficulties involved in the numerical solution of simulation-based nonlinear programming (NLP) problems, especially as occurring in engineering design.

Typically, optimization algorithms rely on simulation codes that are organized as black box objective function generators. A function evaluation may require much computational time and usually do not provide any gradient information, which is required by efficient mathematical optimization methods. Furthermore, iterative procedures, heuristic decisions, low-order approximations of tabular data, spatial and temporal discretization technique or, in general, any kind of numerical method embedded in the simulation code results in noisy objective function evaluation, which rules out the application of Newton-type or, in general, other gradient-based methods. The use of finite differences as approximation to the gradients is not recommended. If, in addition, some optimization variables are integers, the problem complexity grows even further. Even when functions evaluations in analytical form are available, mixed-integer nonlinear programs (MINLP) are challenging optimization problems. MINLPs receive more and more attention from the optimization community. In the context of simulation-based optimization, however, only computationally expensive random search methods like e.g. genetic algorithms are commonly applied. Especially in the presence of integer-valued optimization variables beside of continuous-valued ones and in the presence of constraints that do not reduce to box constraints, it is clear that more efficient solvers are necessary.

For the application considered in this paper, the homogeneity of the magnetic field in the aperture of a superconductive magnet is determined by the geometry of the coil. Especially the position of the coil blocks and the number of turns in each coil block are influencing the quality of the aperture field. The layout of the coils has to obey mechanical constraints such as, e.g., a minimal distance between two adjacent coil blocks. Invoking a separate real-valued optimization for every possible distribution of the integer number of turns over the coil blocks is not feasible by the underlying numerical simulation. Hence, a constrained, mixed-integer nonlinear optimization has to be carried out. The main idea of this paper consists of the application of sequentially improved surrogate functions to approximate the objective function for this design optimization problem. By that, the main barriers for applying well-known MINLP strategies are removed and a branch-and-bound approach can be applied in order to reduce the MINLP problems in each iteration to a number of analytically given and differentiable NLP problems. The NLP subproblems are solved by using a sequential quadratic programming method. The proposed approach is illustrated by an optimization task involving a superconductive-magnet design.

II. Properties of the considered design optimization problem

The function evaluations involve 2D nonlinear magnetostatic field simulations. The partial differential equation

$$-\frac{\partial}{\partial x}\left(\nu\frac{\partial A_z}{\partial x}\right)-\frac{\partial}{\partial y}\left(\nu\frac{\partial A_z}{\partial y}\right)=J_z \qquad (1)$$

where ν is the reluctivity, $A_z(x,y)$ is the z-component of the magnetic vector potential and $J_z(x,y)$ is the z-component of the applied current density, is discretized by linear finite-element (FE) shape functions. Due to symmetry, only a quarter of the magnet cross-section has to be modeled (Fig. 1). The FE solver is equipped with adaptive mesh refinement controlled by a heuristic error estimator based on the locally

stored magnetic energy [1]. This is absolutely necessary to guarantee a reliable function evaluation for *every* geometry suggested by the optimizer. The nonlinearity caused by the ferromagnetic saturation in the iron yoke is resolved by the Newton method. The BH-characteristic has been improved in order to accelerate the convergence of the Newton method and to reduce the numerical noise due to measurement errors [2].

The quality of the design depends on the homogeneity of the magnetic field in the center of the magnet aperture. The radial component B_r of the magnetic flux density at a reference radius r_{ref} is represented by the series expansion, i.e.,

$$B_r\left(r_{\mathrm{ref}},\theta\right) = B_1 \sum_{n=1}^{\infty} b_n \sin(n\theta) + a_n \sin(n\theta)\ . \tag{2}$$

Here, B_1 denotes the magnitude of the vertically oriented dipole magnetic flux density and b_n and a_n are the relative *normal* and *skew* components, evaluated at r_{ref}, respectively [3]. By construction, $b_1\left(r_{\mathrm{ref}}\right)$ equals 1. For a exact dipole field, all other components are 0. Acceptable values for b_n and a_n are in the range of 10^{-4}. These field properties are extracted from the FE solution by evaluating the magnetic vector potential $A_z(r_{\mathrm{ref}},\theta)$ at a circle with the reference radius. The potential distribution is converted into a Fourier series

$$A_z\left(r_{\mathrm{ref}},\theta\right) = \Re\left\{\sum_{n\in\mathcal{S}_0} \underline{c}_n e^{-jn\theta}\right\}\ . \tag{3}$$

The relative normal and skew components follow from evaluating $B_r = \frac{1}{r}\frac{\partial A_z}{\partial r}$ at $r = r_{\mathrm{ref}}$, yielding $b_n = n\Re\{\underline{c}_n\}/\Re\{\underline{c}_1\}$ and $a_n = -n\Im\{\underline{c}_n\}/\Re\{\underline{c}_1\}$. The *field quality factor* is defined by

$$Q = \sqrt{\sum_{n\in\mathcal{S}_b} b_n^2 + \sum_{n\in\mathcal{S}_a} a_n^2} \tag{4}$$

where $\mathcal{S}_b \subset \mathcal{S}_0$ and $\mathcal{S}_a \subset \mathcal{S}_0$ select the relevant components. The optimization goal is the minimization of Q with the geometrical constraints mentioned above. Typically only the continuous valued variables are considered for optimization which describe the azimuthal distance for each of the n_p coils by $\boldsymbol{p}$, with $\boldsymbol{p} \in \mathbb{R}^{n_p}$. Additionally, the optimization algorithm has to decide on the number of turns applied in each of the coil blocks, which determines the size of the individual blocks. These data are represented by integer numbers $\boldsymbol{s}$, with $\boldsymbol{s} \in \mathbb{N}^{n_s}$.

The sum of turns on all coil blocks is fixed, and furthermore a gap of the size of one winding has to be respected between two neighboring coil blocks. These geometric restrictions lead to lower and upper bounds as well as linear constraints on the optimization variables $\boldsymbol{p}$ and $\boldsymbol{s}$, which are summarized by

$$\boldsymbol{p}_l \le \boldsymbol{p} \le \boldsymbol{p}_u, \quad \boldsymbol{s}_l \le \boldsymbol{s} \le \boldsymbol{s}_u, \tag{5}$$

with $\boldsymbol{p}_l, \boldsymbol{p}_u \in \mathbb{R}^{n_p}$, $\boldsymbol{s}_l, \boldsymbol{s}_u \in \mathbb{R}^{n_s}$, and by

$$\boldsymbol{A}(\boldsymbol{p}^T, \boldsymbol{s}^T)^T \le \boldsymbol{b}, \quad \boldsymbol{b} \in \mathbb{R}^{n_b}, \quad \boldsymbol{A} \in \mathbb{R}^{n_b\times(n_p+n_s)}. \tag{6}$$

The resulting set of tuples $(\boldsymbol{p},\boldsymbol{s})$ of feasible design candidates for the device is defined by $\boldsymbol{\Omega}$. Equation (4) provides the simulation based objective function value for a certain combination of $(\boldsymbol{p},\boldsymbol{s})$, which has to minimized for a good design. Finally,

$$\min f(\boldsymbol{p},\boldsymbol{s}) := Q(\boldsymbol{p},\boldsymbol{s}),\ \text{subject to}\ (\boldsymbol{p},\boldsymbol{s}) \in \boldsymbol{\Omega}. \tag{7}$$

defines the resulting mixed integer nonlinear optimization problem.

III. Surrogate optimization for mixed-integer nonlinear problems

The MINLP is summarized in (7). The parameter settings for $\boldsymbol{p}$ and $\boldsymbol{s}$ are supplied to the magnetic-field simulator, which returns the resulting objective function value $f(\boldsymbol{p},\boldsymbol{s})$ obtained as a post-processing result to the optimizer. As already indicated, the real optimization routine is not applied to the original function f but to a surrogate $\hat{f}$ for f. The surrogate function allows to filter the noise introduced by the underlying numerical simulation and allows the relaxation of the discrete variables in $\boldsymbol{s}$.

A. Approximation of a surrogate problem

The approximation of the surrogate problem is based on an extension of the classical approach from Sacks et al. [4], known as Design and Analysis of Computer Experiments (DACE). This extension, proposed in [5], allows to handle not only continuous, real-valued variables but also discrete, integer-valued ones in such a way that the simulation-based objective function is approximated by a stochastic model. The resulting approximation $\hat{f}$ is a two component model,

$$\hat{f}(\boldsymbol{p},\boldsymbol{s}) = \sum_{j=1}^{k} \beta_j h_j(\boldsymbol{p},\boldsymbol{s}) + Z(\boldsymbol{p},\boldsymbol{s}).$$

The first and more global part approximates the global trend of the unknown function f by a linear combination of a vector $\boldsymbol{\beta} \in \mathbb{R}^k$, and a known fixed function $\boldsymbol{h}$, with $\boldsymbol{h} : \mathbb{R}^{n_p} \times \mathbb{R}^{n_s} \to \mathbb{R}^{n_k}$. For the considered application the idea of ordinary kriging is followed with a one dimensional β, and a constant also one dimensional basis function h.

The second part Z guarantees that $\hat{f}$ fits to f for a number of feasible system designs, i.e.,

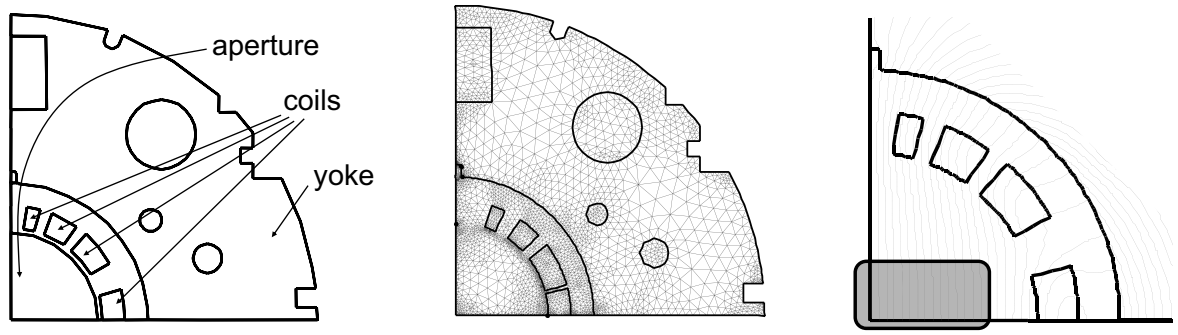
$$\mathcal{B} := \{(\boldsymbol{p}_i,\boldsymbol{s}_i)\}_{i=1,\ldots,n} \subset \boldsymbol{\Omega},$$

and the related objective functions values,

$$f(\boldsymbol{p},\boldsymbol{s}) = \hat{f}(\boldsymbol{p},\boldsymbol{s}), \quad \forall\ (\boldsymbol{p},\boldsymbol{s}) \in \mathcal{B}. \tag{8}$$

This lack-of-fit-part is assumed to be a realization of a stationary Gaussian random function as originally proposed by Sacks et al. [4]. The regression parameter β, as well as the process variance and the correlation parameters for Z, are estimated by maximum likelihood approach, such that they bring a maximal consistency to the present objective function values to which $\hat{f}$ has to fit, as given in (8).

Under the assumption that the approximated function really behaves like a Gaussian random process, the expected mean square error (MSE) of the approximation by DACE gives an estimation of the approximation quality for a certain tuple $(\boldsymbol{p},\boldsymbol{s})$. This information is needed later during the sequential update procedure. The main effects of f should be covered



(a) Parts of the device (b) 2D Mesh (c) Area of interest

Fig. 1. 2D design optimization problem of the location and size of the coil blocks (a), the resulting mesh of a considered design (b), and the visualization of the computed electromagnetic field in the aperture of the magnet (c).

by $\hat{f}$, but it is obvious that $\hat{f}$ is only exact for elements from the set $\mathcal{B}$. For all other feasible tuples $(\boldsymbol{p}, \boldsymbol{s}) \notin \mathcal{B}$, the MSE is larger than zero.

B. Solving a surrogate problem

The approximated surrogate problem carries out a computational cheap, completely analytically given, and differentiable surrogate function $\hat{f}$, defined on a completely real-valued domain $\hat{\mathbf{\Omega}}$, which is the continuous relaxation of $\mathbf{\Omega}$. Therefore, the use of a decomposition method developed for MINLP, such as e.g. branch-and-bound (BB) [6], is made possible. Such methods are normally not applicable to the original objective function because the underlying simulations are often not defined for relaxed integer-valued variables. Furthermore, the surrogate model is not influenced by the noise induced by the numerical simulation into the original objective function and, hence, the step by step generated BB-tree of NLP subproblems can be solved efficiently by sequential quadratic programming methods, as e.g. described in [7]. It also allows to include the explicitly given linear and box constraints from equations (5) and (6) directly into the optimization process on the surrogate problem.

C. Sequential optimization procedure

The often limited, available computational power requires to avoid the simulation of a space-filling set of possible system designs at once. This suggests a more efficient sequential optimization procedure. First, a small initial set of system designs $\mathcal{B}_{in} = \{(\boldsymbol{p}^{(l)}, \boldsymbol{s}^{(l)})\}_{l=1,\ldots,k}$ is selected and simulated in order to generate an initial surrogate optimization problem. To start the iteration, the minimizer $(\boldsymbol{p}^{(*in)}, \boldsymbol{s}^{(*in)})$ of the initial surrogate problem as the next candidate is evaluated by the electromagnetic field simulation and added to $\mathcal{B}_{in}$ to become a new basis $\mathcal{B}_1$ of a new surrogate function $\hat{f}^{(1)}$. This is repeated in each iteration in order to build new surrogate problems by extending the previous basis. But if a minimizer $(\boldsymbol{p}^{(*j)}, \boldsymbol{s}^{(*j)})$ during iteration j is inside an ϵ-ball around the elements of $\mathcal{B}_j$, the process is forced to find a design $(\boldsymbol{p}^{(\diamond j)}, \boldsymbol{s}^{(\diamond j)})$ which maximizes the MSE of $\hat{f}^{(j)}$ in order to get more information about unexplored areas of $\hat{\mathbf{\Omega}}$, respectively $\mathbf{\Omega}$. Another effect of this switching criteria is that the optimization can not stuck into a local minimum. The described procedure ensures that all earlier obtained information as results from computationally expensive simulations is included for the selection of new promising designs during the iterative approximation and optimization procedure. This is done until a stopping criteria is satisfied, in our case, after a limited number of objective function evaluations by the underlying simulation, or when a design is found with an objective function value equal or below prescribed value determined by theoretical consideration about the model.

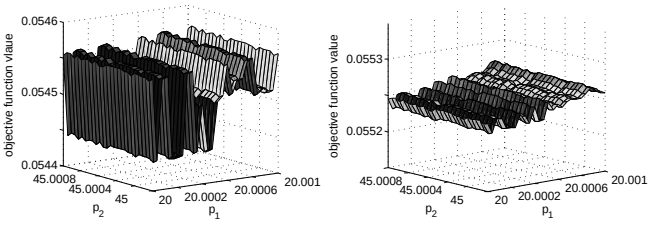
IV. Numerical results

A. General settings

The described approach using surrogate functions is implemented using MATLAB and a DACE toolbox [8], combined with an electromagnetic field simulation software [1]. The optimization problem is invoked for a fixed number of four coil blocks and a total number of 32 turns, equivalent to the variables $\boldsymbol{p} \in \mathbb{R}^3$ and $\boldsymbol{s} \in \mathbb{N}^3$. The number of linear constraints resulting from the geometric requirement given by $\boldsymbol{A}$ and $\boldsymbol{b}$ is 5. The minimal distinction allowed between two considered design candidates controlled by the size of the ϵ-balls introduced in Section 3 is motivated by the manufacturing tolerance of the real device, which is assumed to be met by $\epsilon = 10^{-4}$. During our numerical experiments, it turns out that best found designs of different applied optimization methods without mesh adaptation in the numerical simulation are unstable with regards to small changes in the positions of the coil blocks, which indicates the necessity of mesh adaptation. An impression of the discontinuity in the optimization surface without mesh adaption is given in Fig. 2, where function values of f are plotted for a grid of 26 variations of the second and the third coil by steps of 4ϵ. The resulting change in f is ten times higher without mesh adaptation, and more than ten times higher than the lowest found objective function value.

B. Optimization process results

Fig. 3 illustrates the quality improvement of the magnetic field according to the applied number of simulation calls. The progress of three optimization runs with an Evolutionary Algorithm (EA) shown in Fig. 3. Three expert's guesses for



(a) Without mesh adaption (b) Mesh adaptation applied

Fig. 2. Comparison of the optimization surface smoothness without (a.) and with (b.) one mesh adaption step.

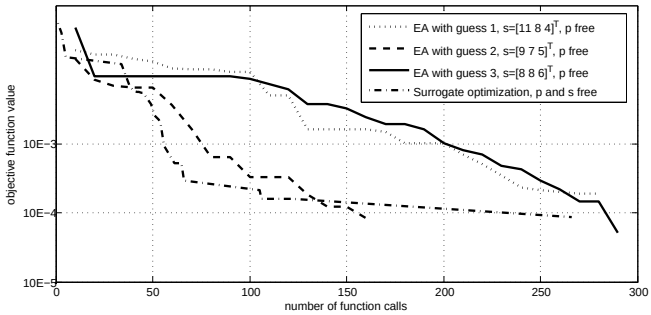
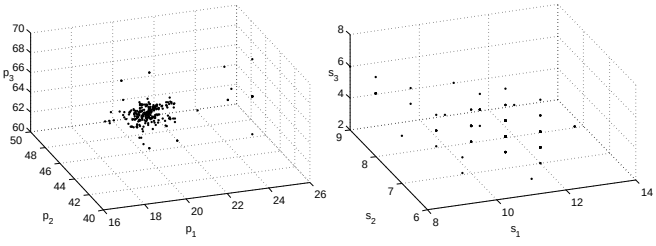


Fig. 3. Progress of three different optimization methods, three runs with an Evolutionary Algorithm, each with a different discrete design and only free continuous design variables, and one run with the proposed surrogate optimization method, with free discrete and free continuous design variables.

the distributions $\boldsymbol{s}$ of the turns over the coil blocks are used to optimize position of the coils given by $\boldsymbol{p}$. Around these three initial expert's guesses the initial set of points $\mathcal{B}_{in}$ for approximation is built. It is done by varying each dimension of each of expert's guesses separately in both directions as proposed in [9]. During 3 out of the 4 different optimization runs a design with an objective function value of less than 10^{-4} is found in less than 300 simulation calls. It is to emphasize that the EA was run on the three dimensional NLP, whereas the surrogate approach was run on a 6 dimensional MINLP.

All generated design candidates, given by tuples $(\boldsymbol{p}, \boldsymbol{s})$, during all iterations of the surrogate optimization approach are plotted in Fig. 4. The finally obtained best design has an discrete part $\boldsymbol{s}$ which was not suggested as one of the expert's guesses and was not a part of a tuple out of the set $\mathcal{B}_{in}$. Further applied approaches of classical design of experiments [10] to



(a) Evaluated variation of $\boldsymbol{p}$ (b) Evaluated variation of $\boldsymbol{s}$

Fig. 4. Different design candidate separated in $\boldsymbol{p}$ and $\boldsymbol{s}$ evaluated during all iterations the proposed MINLP approach by surrogate functions.

generate a spacefilling initial sets $\mathcal{B}_{in}$ like Latin Hypercube sets, grids, or just random sets of points have not carried out any candidate $(\boldsymbol{p}, \boldsymbol{s})$ with an objective function even close to 10^{-4}.

As a further optimization approach, a test version of a commercial EA is applied. This optimization package is able to handle mixed integer nonlinear optimization problems even with linear and nonlinear constraints in its default settings. But the attempts to find results for a comparison with the surrogate optimization approach on the 6 dimensional MINLP problem was not successful. Even after thousands of simulation calls no design of comparable quality is found by this commercial EA. Changes in the parameters settings of the EA have not led to any further improvement.

V. Conclusion

The aperture-field quality of the considered superconductive magnet can be significantly improved on the basis of the presented surrogate optimization approach: The determination of the optimal coil geometry only consumed a acceptably small number of computationally expensive electromagnetic field simulations, especially if it is considered that the applied optimization approach solved a 6 dimensional MINLP problem, in comparison with the EA results of a three dimensional NLP problem obtained by fixing the integer-valued design parameters. An expert's guess is still helpful to start in a region of good candidates for the magnet design. The proposed surrogate technique, however, needs in this application only 3 approximate guesses and does not necessitate the optimization of a large number of optimization problems for each possible combination of the integer-valued design parameters, as is the case for standard optimization methods.

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