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Gradient method with AFEM for parameter-estimation

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Abstract
We consider the adaptive finite element discretization of parameter estimation problems for nonlinear elliptic partial differential equations. The idea is to use a gradient method on the finite-dimensional parameter space for the minimization of the least-squares residual. Since the gradient involves solution of partial differential equations, it is not accesable, and is replaced by an approximation obtained by finite elements. This results into a perturbed gradient method. We use an (a posteriori) error estimator to control the accuracy of the gradient approximation and propose an algorithm, which links the estimator to the progress of the iteration. We show convergence of the algorithm under typical structural assumptions.
Keywords . Adaptive finite element methods, parameter estimation, gradient method.

1. Introduction. We consider parameter estimation for a nonlinear elliptic partial differential equations in a bounded polyhedral domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}_1$,

$$-\operatorname{div}(A(u)\nabla u) = f(u) + b(p) \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega, \tag{1.1}$$

where $f(u), b(p) \in L^2(\Omega)$ and the right-hand side depends smoothly on u and a finite-dimensional parameter $p \in Q = \mathbb{R}^{n_Q}$. The parameter is sought to best fit given data $C^D \in Z = \mathbb{R}^{n_Z}$ in the least-squares sense, minimizing

$$J(p, u) := \frac{1}{2}\sum_{i=1}^{n_Z} R_i(u)^2 + \frac{\alpha_{\text{LS}}}{2}\|p\|^2, \quad R_i(u) := C_i(u) - C_i^D, \tag{1.2}$$

where $C = V \to Z$ is the observation operator (supposed to be linear), R_i is the least-squares residual, and $0 \leq \alpha_{\text{LS}}$. We throughout suppose that this parameter estimation problem is well-defined, i.e., there exists is unique solution p^* depending continuously on data. The latter property amounts in the considered smooth case to have a strictly positive Hessian of the reduced functional $\hat{J}$ in a neighborhood of the solution.

The discretization of the state equation (1.1) by a conforming finite-element method leads to an approximate parameter estimation problem; suppose its solution is p_h^*. In the case of linear state equation (1.1), a priori and a posteriori error estimates for the error in parameter, $\|p^* - p_h^*\|$, have been derived in [1]. These estimates differ from previous estimates in the literature on optimal control problems, since they avoid suboptimal bounds, which typically arise, when the sum of bounds of the energy errors for the state and adjoint variables are used. This allows to have sharper estimates for the parameter error in many cases, see also Lemmas 3.2 and 3.3 below. Moreover, optimal convergence rates of an adaptive finite element method (AFEM) in terms of unknowns (and even work) have been shown in [1].

Our present concern is the generalization of the above-mentioned results to (1.1). In addition, here we wish to consider the problem from an optimization point of view. More precisely, instead of solving

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the optimization problem on a sequence of meshes, we consider a perturbed gradient method for the continuous minimization problem, and interpret discretization as perturbation to the functional and gradient evaluations.

In Section 2 we describe the considered setting based on weak formulations of the different partial differential equations of interest. We discuss the computation of the reduced least-squares functional and its gradient, both on continuous and discrete level. This information is then used in Section 3 in order to obtain error estimators of the functional value and gradient. Since the gradient error is related to the parameter error, we derive estimators as discussed above similar to [1]. The error estimator enables us to propose a perturbed gradient method in Section 4. The idea is to couple the estimator bounding the approximation of the gradient to the norm of the approximated gradient, which measures the progress of the iteration. Under typical assumptions of AFEM theory, we prove that the total error, the weighted sum of the estimator and the continuous functional gap, converge quasi-geometrically. The rate has the typical behavior of a gradient method with respect to the condition number of the function (ratio of the Lipschitz constant of the gradient to the strong convexity parameter). Finally we draw some conclusions in Section 5 and discuss some generalisations.

2. Considered parameter estimation problem. The state equation (1.1) is understood in the weak formulation, written with $V = H^1_0(\Omega)$ as

$$u = u(p) \in V: \ a(u)(v) = l(p)(v) \quad \forall v \in V. \tag{2.1}$$

Here $a : V \times V \to \mathbb{R}$ denotes a smooth (not necessarily bilinear) form. We suppose that it is monotone and Lipschitz-continuous,

$$\begin{cases} a(u)(u-v) - a(v)(u-v) \geq \alpha \left\|u-v\right\|_V^2 \quad \forall u, v \in V, \\ a(u)(v) - a(w)(v) \leq C_a \left\|u-w\right\|_V \left\|v\right\|_V \quad \forall u, v, w \in V. \end{cases} \tag{2.2}$$

We note that monotonicity is equivalent to

$$a'(u)(v,v) \geq \alpha \left\|v\right\|_V^2 \quad \forall u, v \in V. \tag{2.3}$$

By our assumptions, for given $p \in Q$, we have a unique solution $u(p)$ to (2.1) and we can introduce the reduced functional

$$\hat{J}(p) := J(p, u(p)). \tag{2.4}$$

Its gradient can be computes as

$$\langle \nabla \hat{J}(p), q \rangle = \alpha_{\text{LS}} \langle p, q \rangle + l'(p)(q, z(p)), \tag{2.5}$$

where $z \in V$ is the unique solution to

$$z = z(p) \in V: \ a'(u(p))(v, z) = J'_u(p, u(p))(v) \quad \forall v \in V, \tag{2.6}$$

see for example [2]. We make the hypothesis of μ-convexity of the reduced functional, which means that there exists $\mu > 0$, such that

$$\langle \nabla^2 \hat{J}(p) q, q \rangle \geq \mu \left\|q\right\|^2 \quad \forall q \in Q. \tag{2.7}$$

Let $V_h \subset V$ be a conforming finite-element subspace, where $h \in \mathcal{H}$ is an element of a given shape-regular family of simplicial meshes $\mathcal{H}$. Then $u_h = u_h(p)$ is defined by the discrete problem

$$u_h \in V_h: \ a(u_h)(v) = l(p)(v) \quad \forall v \in V_h, \tag{2.8}$$

and

$$z_h = z_h(p) \in V_h: \ a'(u_h(p))(v, z_h) = J'_u(p, u_h(p))(v) \quad \forall v \in V_h. \tag{2.9}$$

Similar to (2.12) we have for the discrete reduced functional $\hat{J}_h(p) := J(p, u_h(p))$ that

$$\langle \nabla \hat{J}_h(p), q \rangle = \alpha_{\text{LS}} \langle p, q \rangle + l'(p)(q, z_h(p)). \tag{2.10}$$

Note that, in contrast to the infinite-dimensional case, (2.7) does in general not require $\alpha_{\text{LS}} > 0$.

Instead of (2.1) we consider the adjoint equations for $z^{(i)} = z^{(i)}(p)$ (for $1 \leq i \leq n_Z$)

$$z^{(i)} \in V: \ a'(u(p))(v, z^{(i)}) = C_i(v) \quad \forall v \in V, \tag{2.11}$$

which leads to $z = \sum_{i=1}^{n_Z} R_i(u) z^{(i)}$ and we have

$$\langle \nabla \hat{J}(p), q \rangle = \alpha_{\mathrm{LS}} \langle p, q \rangle + \sum_{i=1}^{n_Z} R_i(u) l'(p)(q, z^{(i)}). \tag{2.12}$$

A gradient step for the minimization of the discrete functional $\nabla \hat{J}_h(p)$ starting from p_k can now be performed by solving the discrete state equation (2.8) and the discrete adjoint equations for $z_h^{(i)} = z_h^{(i)}(p)$

$$z_h^{(i)} \in V_h : \; a'(u_h(p))(v, z_h^{(i)}) = C_i(v) \quad \forall v \in V_h. \tag{2.13}$$

We can then perform a step of the gradient method,

$$\langle p_{k+1}, q \rangle = \langle (1 - t_k \alpha_{\mathrm{LS}}) p_k, q \rangle + t_k \sum_{i=1}^{n_Z} R_i(u_h(p_k)) \left(l'(p)(q, z_h^{(i)}) - a'(p_k)(q, z_h^{(i)}(p_k)) \right) \quad \forall q \in Q, \tag{2.14}$$

where t_k is the step size.

Finally, we state that μ-convexity of the reduced functional leads to the following bound for the parameter error with

Lemma 2.1.

$$\|p^* - p_h^*\| \leq \mu^{-\frac{1}{2}} \left\| \nabla \hat{J}(p_h^*) - \nabla \hat{J}_h(p_h^*) \right\|. \tag{2.15}$$

An alternative formula for the gradient of the reduced functional relies on the solution to the tangent problem for $u' = u'(p)(q)$

$$u' \in V : \; a'(u(p))(u', v) = l'(p)(q, v) \quad \forall v \in V. \tag{2.16}$$

We then have

$$\langle \nabla \hat{J}(p), q \rangle = \alpha_{\mathrm{LS}} \langle p, q \rangle + \sum_{i=1}^{n_Z} R_i(u) C_i(u'(p)(q)). \tag{2.17}$$

Let $(e_j)_{1 \leq j \leq n_Q}$ be a basis of Q. Then we have $u'(p)(q) = \sum_{j=1}^{n_Q} u^{(j)}(p) q_j$, where, with $l'_j(p, v) = l'(p)(e_j, v)$, and

$$u^{(j)}(p) \in V : \; a'(u(p))(u^{(j)}(p), v) = l'_j(p)(v) \quad \forall v \in V. \tag{2.18}$$

The analogous formula holds for the gradient of the discrete reduced functional by means of

$$u_h^{(j)}(p) \in V : \; a'(u(p))(u_h^{(j)}(p), v) = l'_j(p)(v) \quad \forall v \in V_h. \tag{2.19}$$

We have the following Céa-type results.

Lemma 2.2.

$$\begin{cases} \|u - u_h\|_V \leq \dfrac{C_a}{\alpha} \inf_{v_h \in V_h} \|u - v_h\|_V \,, \\ \left\| z^{(i)} - z_h^{(i)} \right\|_V \leq \dfrac{C_a}{\alpha} \inf_{v_h \in V_h} \left\| z^{(i)} - v_h \right\|_V + \dfrac{C'_a |||C_i|||}{\alpha^2} \|u - u_h\|_V \,, \\ \left\| u^{(j)} - u_h^{(j)} \right\|_V \leq \dfrac{C_a}{\alpha} \inf_{v_h \in V_h} \left\| u^{(j)} - v_h \right\|_V + \dfrac{C'_a |||l'(p)|||}{\alpha^2} \|u - u_h\|_V \,. \end{cases} \tag{2.20}$$

Proof: By (2.2)

$$\begin{aligned} \alpha \|u - u_h\|_V^2 \leq & a(u)(u - u_h) - a(u_h)(u - u_h) \\ = & a(u)(u - v_h) - a(u_h)(u - v_h) \leq C_a \|u - u_h\| \|u - v_h\|_V \,. \end{aligned}$$

With $v = z^{(i)} - z_h^{(i)}$

$$\begin{aligned} \alpha \left\| z^{(i)} - z_h^{(i)} \right\|_V^2 \leq & a'(u_h)(z^{(i)} - z_h^{(i)}, v) = a'(u)(z^{(i)}, v) - a'(u_h)(z_h^{(i)}, v) + a'(u_h)(z^{(i)}, v) - a'(u)(z^{(i)}, v) \\ \leq & a'(u)(z^{(i)}, v - v_h) - a'(u_h)(z_h^{(i)}, v - v_h) + C'_a \|u - u_h\|_V \left\| z^{(i)} \right\|_V \|v\|_V \\ \leq & C_a \left\| z^{(i)} - z_h^{(i)} \right\| \|v - v_h\| + C'_a \|u - u_h\|_V \frac{|||C_i|||}{\alpha} \left\| z^{(i)} - z_h^{(i)} \right\|_V \,. \end{aligned}$$

The last inequality is similar. □

3. A posteriori error estimation. For a given mesh $h \in \mathcal{H}$, we denote the set of cells by $\mathcal{K}_h$. For illustration, we suppose that the right-hand side is of the form (1.1) and $C_i(u) = \int_\Omega g_i u$ with $g_i \in L^2(\Omega)$ and $l'_j(p) \in L^2(\Omega)$. Next we define the error estimators

$$\rho_h^2(u_h) = \sum_{K\in\mathcal{K}_h} \rho_K^2(u_h), \quad \rho_h^2(z_h) = \sum_{K\in\mathcal{K}_h} \rho_K^2(z_h), \quad \rho_h^2(u'_h) = \sum_{K\in\mathcal{K}_h} \rho_K^2(u'_h)$$

$$\rho_K^2(u_h) = h_K^2 \left\|f(u) + l(p) + \operatorname{div}(A(u)\nabla u_h)\right\|_K^2 + \frac{h_K}{2}\left\|[A(u)\nabla u_h \cdot n_K]\right\|_{\partial K\setminus\partial\Omega},$$

$$\rho_K^2(z_h^{(i)}) = h_K^2 \left\|g_i + f'(u_h) + \operatorname{div}(A'(u_h)\nabla z_h^{(i)})\right\|_K^2 + \frac{h_K}{2}\left\|\left[A'(u_h)\nabla z_h^{(i)} \cdot n_K\right]\right\|_{\partial K\setminus\partial\Omega},$$

$$\rho_K^2(u_h^{(j)}) = h_K^2 \left\|f'(u_h) + l'_j(p) + \operatorname{div}(A'(u_h)\nabla u_h^{(j)})\right\|_K^2 + \frac{h_K}{2}\left\|\left[A'(u_h)\nabla u_h^{(j)} \cdot n_K\right]\right\|_{\partial K\setminus\partial\Omega}.$$

We have the following a posteriori bounds.

Lemma 3.1.

$$\begin{cases} \|u-u_h\|_V \le \dfrac{C_{\text{int}}}{\alpha}\rho_h(u_h), \\ \left\|z^{(i)} - z_h^{(i)}\right\|_V \le \dfrac{C_{\text{int}}}{\alpha}\rho_h(z_h^{(i)}) + \dfrac{|||C_i|||C'_a C_{\text{int}}}{\alpha^2}\rho_h(u_h), \\ \left\|u^{(j)} - u_h^{(j)}\right\|_V \le \dfrac{C_{\text{int}}}{\alpha}\rho_h(u_h^{(j)}) + \dfrac{|||b'_j(p)|||C'_a C_{\text{int}}}{\alpha^2}\rho_h(u_h). \end{cases} \tag{3.1}$$

Proof: By (2.2) with $v := u - u_h$

$$\alpha\|u-u_h\|_V^2 \le a(u)(v) - a(u_h)(v) = a(u)(v-v_h) - a(u_h)(v-v_h) = l(p)(v-v_h) - a(u_h)(v-v_h).$$

Then integration by parts and appropriate interpolation give the result. See [3, 4, 5] for details. With $v = z^{(i)} - z_h^{(i)}$

$$\begin{aligned}\alpha\left\|z^{(i)} - z_h^{(i)}\right\|_V^2 \le& a'(u_h)(v, z^{(i)} - z_h^{(i)}) = a'(u)(v,z^{(i)}) - a'(u_h)(v,z_h^{(i)}) + a'(u_h)(v,z^{(i)}) - a'(u)(v,z^{(i)})\\ \le& C_i(v-v_h) - a'(u_h)(z_h^{(i)}, v-v_h) + C'_a\|u-u_h\|_V\left\|z^{(i)}\right\|_V\|v\|_V\\ \le& C_{\text{int}}\rho_h(z_h^{(i)})\|v\|_V + \frac{|||C_i|||C'_a C_{\text{int}}}{\alpha}\rho_h(u_h)\|v\|_V\end{aligned}$$

since

$$\alpha\left\|z^{(i)}\right\|_V^2 \le a'(u)(z^{(i)}, z^{(i)}) = C_i(z^{(i)}) \le |||C_i|||\left\|z^{(i)}\right\|_V.$$

The last inequality is similar. □

Lemma 3.2. ***(Error in functional)*** *We have*

$$\hat{J}(p) - \hat{J}_h(p) \le \sum_{i=1}^{n_Z} E_i(E_i + R_i(u_h)), \quad E_i := \frac{C_{\text{int}}^2}{\alpha}\rho_h(u_h)\left(\rho(z_h^{(i)}) + \frac{C'_a|||C_i|||}{2\alpha^2}\rho_h(u_h)\right) \tag{3.2}$$

Proof: We have for any $v \in V_h$

$$0 = a(u)(v) - a(u_h)(v) = \int_0^1 a'(u_h + t(u-u_h))(u-u_h, v)\,dt,$$

so

$$a'(u_h)(u-u_h, v) = \int_0^1 \left(a'(u_h) - a'(u_h + t(u-u_h))\right)(u-u_h, v) \le \frac{C'_a}{2}\|u-u_h\|^2\|v\|. \tag{3.3}$$

With $v := u - u_h$ and (3.3)

$$\begin{aligned}C_i(u) - C_i(u_h) =& a'(u)(u-u_h, z^{(i)}) = a'(u)(u-u_h, z^{(i)}) - a'(u_h)(u-u_h, z_h^{(i)}) + a'(u_h)(u-u_h, z_h^{(i)})\\ \le& C_i(v-v_h) - a'(u_h)(v-v_h, z_h^{(i)}) + \frac{C'_a}{2}\|u-u_h\|^2\left\|z_h^{(i)}\right\|\\ \le& C_{\text{int}}\rho(z_h^{(i)})\|v\|_V + \frac{C'_a\|C_i\|}{2\alpha}\|u-u_h\|^2.\end{aligned}$$

Then with (3.1)

$$C_i(u) - C_i(u_h) \leq \frac{C_{\text{int}}^2}{\alpha}\rho_h(u_h)\left(\rho(z_h^{(i)}) + \frac{C_a'|||C_i|||}{2\alpha^2}\rho_h(u_h)\right) \tag{3.4}$$

$$\begin{aligned}\hat{J}(p) - \hat{J}_h(p) =& \frac{1}{2}\sum_{i=1}^{n_Z}\left(R_i^2(u) - R_i^2(u_h)\right) = \frac{1}{2}\sum_{i=1}^{n_Z}\left(R_i(u) - R_i(u_h)\right)^2 + \sum_{i=1}^{n_Z}\left(R_i(u) - R_i(u_h)\right)R_i(u_h)\\ =& \frac{1}{2}\sum_{i=1}^{n_Z}\left(C_i(u) - C_i(u_h)\right)\left(C_i(u) - C_i(u_h) + 2R_i(u_h)\right).\end{aligned}$$

□

Lemma 3.3. ***(Error in gradient)*** *We have with*

$$E_i := \rho(z_h^{(i)}) + \frac{C_a'|||C_i|||}{2\alpha^2}\rho_h(u_h), \quad F := \left(\sum_{j=1}^{n_Q}\left(\rho_h(u_h^{(j)}) + \frac{|||l_j'(p)|||C_a'}{\alpha}\rho_h(u_h)\right)^2\right)^{\frac{1}{2}}$$

$$\left\|\nabla\hat{J}(p) - \nabla\hat{J}_h(p)\right\| \leq \frac{C_{\text{int}}^2}{\alpha}\sum_{i=1}^{n_Z}E_i\left(\rho_h(u_h)|||l'(p)||||||C_i||| + R_i(u_h)F\right). \tag{3.5}$$

Remark 3.1. *Both error estimates, (3.2) and (3.5), have a quadratic behavior, since they consist of sums of products of the different residual estimators.*

Proof: We have from (2.17) with $u' = u'(p)(q)$ and $u_h' = u_h'(p)(q)$

$$\begin{aligned}\langle\nabla\hat{J}(p) - \nabla\hat{J}_h(p), q\rangle =& \sum_{i=1}^{n_Z}\left(R_i(u)C_i(u') - R_i(u_h)C_i(u_h'))\right)\\ =& \sum_{i=1}^{n_Z}\left((C_i(u) - C_i(u_h))C_i(u') + R_i(u_h)(C_i(u') - C_i(u_h'))\right)\end{aligned}$$

For the first term we have with

$$\alpha\left\|u'\right\|_V^2 \leq a'(u)(u', u') = l'(p)(q, u') \leq |||l'(p)|||\left\|q\right\|\left\|u'\right\|_V.$$

and (3.4)

$$(C_i(u) - C_i(u_h))C_i(u') \leq \frac{C_{\text{int}}^2}{\alpha}\rho_h(u_h)\left(\rho(z_h^{(i)}) + \frac{C_a'|||C_i|||}{2\alpha^2}\rho_h(u_h)\right)|||l'(p)|||C_i||||||\left\|q\right\|.$$

For the second term similarly as before with $v = u^{(j)} - u_h^{(j)}$

$$\begin{aligned}C_i(u^{(j)}) - C_i(u_h^{(j)}) =& a'(u)(u^{(j)} - u_h^{(j)}, z^{(i)}) = a'(u)(v, z^{(i)}) - a'(u_h)(v, z_h^{(i)}) + a'(u_h)(v, z_h^{(i)})\\ \leq& C_i(v - v_h) - a'(u_h)(v - v_h, z_h^{(i)}) + \frac{C_a'}{2}\left\|u - u_h\right\|\left\|v\right\|\left\|z_h^{(i)}\right\|\\ \leq& C_{\text{int}}\rho(z_h^{(i)})\left\|v\right\|_V + \frac{C_a'|||C_i|||C_{\text{int}}}{2\alpha^2}\rho_h(u_h)\left\|v\right\|.\end{aligned}$$

Using (3.1) we get

$$C_i(u^{(j)}) - C_i(u_h^{(j)}) \leq \frac{C_{\text{int}}^2}{\alpha}\left(\rho(z_h^{(i)}) + \frac{C_a'|||C_i|||}{2\alpha^2}\rho_h(u_h)\right)\left(\rho_h(u_h^{(j)}) + \frac{|||l_j'(p)|||C_a'}{\alpha}\rho_h(u_h)\right)$$

and

$$C_i(u') - C_i(u_h') \leq \frac{C_{\text{int}}^2}{\alpha}\left(\rho(z_h^{(i)}) + \frac{C_a'|||C_i|||}{2\alpha^2}\rho_h(u_h)\right)\left(\sum_{j=1}^{n_Q}F_j^2\right)^{\frac{1}{2}}\left\|q\right\|.$$

□

4. Perturbed gradient method. In this section, we use the notation of optimization, replacing $\hat{J}$ by f, P by X and p by x. So we consider a perturbed gradient method of the form

$$x_{k+1} = x_k - t_k g_k \tag{4.1}$$

for the unconstrained minimization problem

$$\min \{ f(x) \mid x \in X \}, \tag{4.2}$$

where $f : X \to \mathbb{R}$ is a μ-convex function with L-Lipschitz gradient, i.e.

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|x - y\|^2, \quad \|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|. \tag{4.3}$$

In each step of the iteration, only an approximation f_k of f is known (which corresponds for our parameter estimation problem to the reduced functional on a finite-element sub-space V_k), and $g_k = \nabla f_k(x_k)$.

To be more precise, let $\mathcal{H}$ be a lattice of meshes with ordering $h' < h$ if h' is a refinement of h. We suppose to have an error estimator η_h and a refinement algorithm $\mathcal{R} : \mathcal{H} \to \mathcal{H}$ satisfying

$$\|\nabla f(x) - \nabla f_h(x)\| \leq \eta_h(x) \tag{4.4}$$

and with $q_{\mathcal{R}} < 1$ for $h' = \mathcal{R}(h)$

$$\eta_{h'}(x) \leq q_{\mathcal{R}} \eta_h(x), \quad \eta_h^2(x) \leq \eta_h^2(y) + C_S \|x - y\|^2. \tag{4.5}$$

Remark 4.1. *For simpler computations, we suppose the constant in the upper bound (4.4) to be one. In comparison to the preceding section, this requires proper scaling of the error estimator. Following [6], we do not suppose to have a lower bound, but instead decrease of the estimator under refinement. This typically holds for residual-type estimators of the above form, see also [7].* We consider the following algorithm with constant step $t_k = 1/L$.

Algorithm 1 GM with constant step-size

Inputs: $x_0 \in X$, $\varepsilon > 0$, $0 < \lambda < \frac{1}{2}$, $h_0 \in \mathcal{H}$, and $L > 0$. Set $k = 0$.
(1) $g_k := \nabla f_{h_k}(x_k)$.
(2) **if** $\eta_{h_k}(x_k) + \|g_k\| \leq \sqrt{2\varepsilon\mu}$ **then** STOP
(3) **ELSE IF** $\eta_{h_k}(x_k) > \lambda \|g_k\|$ $h_{k+1} = \mathcal{R}(h_k)$
$x_{k+1} = x_k$ $h_{k+1} = h_k$
$x_{k+1} = x_k - \frac{1}{L} g_k$
(4) Increment k and go to (1).

Remark 4.2. *The algorithm performs a gradient step if $\eta_{h_k}(x_k) \leq \lambda \|g_k\|$. This condition controls the approximation of the gradient thanks to (4.4). It is similar to the angle condition in the classical analysis of the gradient method [8].* The algorithm terminates thanks to Proposition 4.1 below. We have the following justification of the stopping criterium.

Lemma 4.1. *If the algorithm stops we have $f(x_k) - f(x^*) \leq \varepsilon$ and $\|x_k - x^*\| \leq \sqrt{2\varepsilon/\mu}$.*

Proof: Let $q(y) := f(x_k) + \langle \nabla f(x_k), y - x_k \rangle + \frac{\mu}{2} \|y - x_k\|^2$. Then $\operatorname{argmin} q = x_k - \frac{1}{\mu} \nabla f(x_k)$ and $q^* = \min q = f(x_k) - \frac{1}{2\mu} \|\nabla f(x_k)\|^2$. By μ-convexity (4.3) we have $f(y) \geq q(y)$ for for all $y \in X$. Then

$$f(x_k) - f(x^*) \leq f(x_k) - q(x^*) \leq f(x_k) - q^* = \frac{1}{2\mu} \|\nabla f(x_k)\|^2 \leq \frac{1}{2\mu} \left(\|g_k\| + \|\nabla f(x_k) - g_k\| \right)^2.$$

We conclude by (4.4). We also have

$$\mu \|x_k - x^*\|^2 \leq \langle \nabla f(x_k) - \nabla f(x^*), x_k - x^* \rangle \leq \|\nabla f(x_k)\| \|x_k - x^*\|.$$

giving the second bound. □

Lemma 4.2. *If $\eta_{h_k}(x_k) \leq \lambda \|g_k\|$ we have*

$$f(x_{k+1}) \leq f(x_k) - \frac{1 - 2\lambda}{2L} \|g_k\|^2 \tag{4.6}$$

and

$$\eta^2_{h_{k+1}}(x_{k+1}) \leq q_{\mathcal{R}}\eta^2_{h_k}(x_k) + \left((1-q_{\mathcal{R}})\lambda^2 + \frac{C_{\mathrm{S}}}{L^2}\right)\|g_k\|^2. \tag{4.7}$$

In addition, if x^* is a minimizer we set $\Delta f_k := f(x_k) - f(x^*)$. Then for $0 < \theta < \frac{1}{2} - \lambda$

$$\Delta f_{k+1} \leq (1-\theta)\Delta f_k + \frac{\theta L}{2}\left(\|x_k - x^*\|^2 - \|x_{k+1}-x^*\|^2\right) + \frac{\theta}{\mu}\eta^2_{h_k}(x_k) - \frac{1-2\lambda-2\theta}{2L}\|g_k\|^2. \tag{4.8}$$

Proof: We first note that with (4.4) we have

$$\|\nabla f(x_k)\| \leq \|g_k\| + \|\nabla f(x_k) - g_k\| \leq (1+\lambda)\|g_k\|$$
$$\|g_k\| \leq \|\nabla f(x_k)\| + \|\nabla f(x_k) - g_k\| \leq \|\nabla f(x_k)\| + \lambda\|g_k\|$$

so

$$(1-\lambda)\|g_k\| \leq \|\nabla f(x_k)\| \leq (1+\lambda)\|g_k\|. \tag{4.9}$$

By (4.3) we have

$$\begin{aligned}
f(x_{k+1}) - f(x_k) \leq& \langle \nabla f(x_k), x_{k+1}-x_k\rangle + \frac{L}{2}\|x_{k+1}-x_k\|^2\\
=& -\frac{1}{L}\langle \nabla f(x_k), g_k\rangle + \frac{1}{2L}\|g_k\|^2\\
=& -\frac{1}{2L}\left(\|g_k\|^2 + \|\nabla f(x_k)\|^2 - \|\nabla f(x_k)-g_k\|^2\right) + \frac{1}{2L}\|g_k\|^2\\
\leq& -\frac{1}{2L}\left(\|g_k\|^2 + (1-\lambda)^2\|g_k\|^2 - \lambda^2\|g_k\|^2\right) + \frac{1}{2L}\|g_k\|^2\\
\leq& -\frac{1}{L}(1-\lambda)\|g_k\|^2 + \frac{1}{2L}\|g_k\|^2 = -\frac{1-2\lambda}{2L}\|g_k\|^2.
\end{aligned}$$

Since in case $\eta_{h_k}(x_k) \leq \lambda\|g_k\|$ we have $h_{k+1} = h_k$ we get from (4.5)

$$\begin{aligned}
\eta^2_{h_{k+1}}(x_{k+1}) =& \eta^2_{h_k}(x_{k+1}) \leq \eta^2_{h_k}(x_k) + C_{\mathrm{S}}\|x_{k+1}-x_k\|^2\\
\leq& q_{\mathcal{R}}\eta^2_{h_k}(x_k) + (1-q_{\mathcal{R}})\lambda^2\|g_k\|^2 + C_{\mathrm{S}}\|x_{k+1}-x_k\|^2 = q_{\mathcal{R}}\eta^2_{h_k}(x_k) + \left((1-q_{\mathcal{R}})\lambda^2 + \frac{C_{\mathrm{S}}}{L^2}\right)\|g_k\|^2.
\end{aligned}$$

Further by (4.3) we have

$$\begin{aligned}
f(x_k) - f(x^*) \leq& \langle \nabla f(x_k), x_k - x^*\rangle - \frac{\mu}{2}\|x_k - x^*\|^2\\
=& \langle g_k, x_k - x^*\rangle - \frac{\mu}{2}\|x_k-x^*\|^2 + \langle \nabla f(x_k) - g_k, x_k - x^*\rangle\\
=& \frac{L}{2}\left(\frac{1}{L^2}\|g_k\|^2 + \|x_k-x^*\|^2 - \|x_{k+1}-x^*\|^2\right) - \frac{\mu}{2}\|x_k-x^*\|^2 + \langle \nabla f(x_k)-g_k, x_k-x^*\rangle\\
\leq& \frac{L}{2}\left(\|x_k-x^*\|^2 - \|x_{k+1}-x^*\|^2\right) + \frac{1}{L}\|g_k\|^2 + \frac{1}{\mu}\eta^2_{h_k}(x_k).
\end{aligned}$$

Adding θ-times the last inequality to (4.6) yields the result. □

We conclude from (4.6) and (4.7) that under the hypothesis of Lemma 4.2 we have $\alpha > 0$ sufficiently small such that there exists $c_0 > 0$ satisfying for ant $q_{\mathcal{R}} \leq q'_{\mathcal{R}} < 1$

$$f(x_{k+1}) - f(x_k) + \alpha\eta^2_{h_{k+1}}(x_{k+1}) + c_0\|g_k\|^2 \leq \alpha q'_{\mathcal{R}}\eta^2_{h_k}(x_k). \tag{4.10}$$

This is the basic estimate to obtain the following result.

Proposition 4.1. *Let $\{x \mid f(x) \leq f(x_0)\}$ be bounded. The sequence generated by the gradient method converges towards the unique solution x^*.*

Proof: We show that in the first case of the algorithm an estimate similar to (4.10) still holds. In this case we have $f(x_{k+1}) = f(x_k)$, reduction (4.5), and $\|g_k\| \leq \lambda^{-1}\eta_{h_k}(x_k)$, such that

$$\eta^2_{h_{k+1}}(x_{k+1}) + c_0\|g_k\|^2 \leq q_{\mathcal{R}}\eta^2_{h_k}(x_k) + \frac{c_0}{\lambda^2}\eta^2_{h_k}(x_k) \leq q'_{\mathcal{R}}\eta^2_{h_k}(x_k)$$

with $q_{\mathcal{R}} \leq q'_{\mathcal{R}} < 1$ if $c_0 > 0$ sufficiently small. So we have (4.10) in both cases.

Summing up (4.10) from n to $N > n$ leads to

$$f(x_{N+1}) + \alpha q'_{\mathcal{R}} \eta^2_{h_{N+1}}(x_{N+1}) + \alpha(1 - q'_{\mathcal{R}}) \sum_{k=n+1}^{N+1} \eta^2_{h_k}(x_k) + c_0 \sum_{k=n}^{N} \|g_k\|^2 \leq f(x_n) + \alpha q'_{\mathcal{R}} \eta^2_{h_n}(x_n).$$

Since the right-hand side is independent of N we can pass to the limit $N \to \infty$ and obtain $\lim_{k\to\infty} \|g_k\| = 0$ and $\lim_{k\to\infty} \eta_{h_k}(x_k) = 0$. Then by (4.4)

$$\|\nabla f(x_k)\| \leq \|g_k\| + \|\nabla f(x_k) - g_k\| \leq \|g_k\| + \eta_{h_k}(x_k) \to 0 \quad (k \to \infty) .$$

□

Finally we consider the convergence rate of the algorithm.

Theorem 4.1. *Let $\kappa_f := L/\mu$ and $E_k := \Delta f_k + \frac{1}{L}\eta^2_{h_k}(x_k)$. Then there exist $C > 0$ and $0 < \rho < 1$ such that*

$$E_{n+k} \leq C\rho^k E_n \quad \forall k, n \in \mathbb{N}, \tag{4.11}$$

where $\rho = 1 - 1/C$ and $C \leq C_0\kappa_f$ with $C_0 > 0$ independent of κ_f.

Remark 4.3. *Although we know by (4.6) that the functional is monotone, the total error can in general not be expected to have the same behavior. This is reflected in (4.11), where a quasi-geometric convergence is stated. The dependance of ρ on κ_f is optimal, see [9].*

Proof: In case $\eta_{h_k}(x_k) \leq \lambda \|g_k\|$, we use (4.8) (4.7) and (4.6).

$$\begin{aligned}\Delta f_{k+1} + \frac{1}{L}\eta^2_{h_{k+1}}(x_{k+1}) \leq& (1-\theta)\Delta f_k + \left(q_{\mathcal{R}} + \frac{\theta L}{\mu}\right)\frac{1}{L}\eta^2_{h_k}(x_k) + \\ & \frac{\theta L}{2}\left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2\right) + B\left(f(x_k) - f(x_{k+1})\right),\end{aligned}$$

with

$$B := \frac{1}{L}\left((1-q_{\mathcal{R}})\lambda^2 + \frac{C_{\mathrm{S}}}{L^2}\right)\frac{2L}{1-2\lambda} = 2\frac{(1-q_{\mathcal{R}})\lambda^2 + C_{\mathrm{S}}/L^2}{(1-2\lambda)}.$$

In case $\eta_{h_k}(x_k) > \lambda \|g_k\|$ we have

$$\Delta f_{k+1} + \frac{1}{L}\eta^2_{h_{k+1}}(x_{k+1}) \leq (1-\theta)\Delta f_k + \theta\left(f(x_k) - f(x^*)\right) + q_{\mathcal{R}}\frac{1}{L}\eta^2_{h_k}(x_k).$$

By (4.3), Young's inequality and (4.9)

$$f(x_k) - f(x^*) \leq \langle \nabla f(x_k), x_k - x^*\rangle - \frac{\mu}{2}\|x_k - x^*\|^2 \leq \frac{1}{2\mu}\|\nabla f(x_k)\|^2 \leq \frac{(1+\lambda)^2}{2\mu}\|g_k\|^2,$$

such that with $\|g_k\|^2 \leq \eta^2_{h_k}(x_k)/\lambda^2$

$$\Delta f_{k+1} + \frac{1}{L}\eta^2_{h_{k+1}}(x_{k+1}) \leq (1-\theta)\Delta f_k + \left(q_{\mathcal{R}} + \frac{\theta(1+\lambda)^2 L}{2\mu\lambda^2}\right)\frac{1}{L}\eta^2_{h_k}(x_k).$$

Let

$$q' := q_{\mathcal{R}} + \theta \max\left\{\frac{L}{\mu}, \frac{(1+\lambda)^2 L}{2\mu\lambda^2}\right\} = q_{\mathcal{R}} + \theta\kappa_f\frac{(1+\lambda)^2}{2\lambda^2},$$

where we have used $(1+\lambda)^2 \geq 2\lambda^2$. For θ small enough we have $q' < 1$ and then with $\tilde{q} := \max\{(1-\theta), q'\}$

$$\Delta f_{k+1} + \frac{1}{L}\eta^2_{h_{k+1}}(x_{k+1}) \leq \tilde{q}\left(\Delta f_k + \frac{1}{L}\eta^2_{h_k}(x_k)\right) + \frac{\theta L}{2}\left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2\right) + B\left(f(x_k) - f(x_{k+1})\right).$$

We know already that $\eta^2_{h_k}(x_k) \to 0$ and $x_k \to x^*$, so summing up the last inequality from n to $N > n$ and letting $N \to \infty$ we find

$$\begin{aligned}(1-\tilde{q})\sum_{k=n+1}^{\infty} A_k \leq& \tilde{q}A_n + \frac{\theta L}{2}\|x_n - x^*\|^2 + B\left(f(x_n) - f(x^*)\right) \\ \leq& \tilde{q}A_n + \left(\frac{\theta L}{\mu} + B\right)\left(f(x_n) - f(x^*)\right),\end{aligned}$$

such that

$$\sum_{k=n+1}^{\infty} A_k \leq C A_n,$$

with $C := \left(\tilde{q} + \frac{\theta L}{\mu} + B\right)/(1-\tilde{q})$.

With $S_n := \sum_{k=n}^{\infty} A_k$, the last inequality reads

$$S_{n+1} \leq C\left(S_n - S_{n+1}\right) \quad \Rightarrow \quad S_{n+k} \leq \rho^k S_n, \quad \rho := \frac{C}{C+1}.$$

And finally

$$A_{n+k} \leq S_{n+k} \leq \rho^{k-1} S_{n+1} \leq \frac{C}{\rho}\rho^k A_n = (C+1)\rho^k A_n.$$

Finally we analyze the dependance of C on κ_f. Let $\theta := \frac{(1-q_{\mathcal{R}})\lambda^2)}{\kappa_f(1+\lambda)^2}$, which is possible if $\kappa_f \geq 1$ is large. It turns out that $\tilde{q} = 1-\theta$ and then

$$C = \frac{\tilde{q} + \frac{\theta L}{\mu} + B}{1-\tilde{q}} = \frac{1-\theta+\kappa_f\theta+B}{\theta} \leq \frac{1+\kappa_f\theta+2\frac{(1-q_{\mathcal{R}})\lambda^2+C_{\mathrm{S}}}{(1-2\lambda)}}{\theta} \leq C_0\kappa_f,$$

with C_0 depending on λ, $q_{\mathcal{R}}$, and C_{S}, but not on κ_f. □

5. Conclusion. In this contribution, we have shown how adaptive discretization of PDE-constrained minimization in form of parameter identification can be cast into the framework of a perturbed gradient method. The important ingredient is an error estimator for the error in gradient. It is used to adjust the finite element discretization during the iteration and also allows for a simple stopping criterion of the algorithm, which is shown to have the typical convergence rate of a gradient method.

In contrast to [1], we have not touched the crucial theoretical question of convergence rates in terms of unknowns. One would like to ensure that the parameter error $f(x_k) - f(x^*)$ behaves like N_k^{-s}, where N_k is the sum of dimensions of all finite element spaces used up to iteration k, and $s > 0$ is any possible rate.

Further possible extensions are the generalization to adaptive step-sizes and the incomplete solution of the discrete state equation. Adaptive step-sizes are important to treat nonlinearities that are only locally Lipschitz-continuous [10], and avoid the explicit knowledge of a Lipschitz-constant. Although the presented algorithm avoids solution of the optimization problem on each finite element space, it supposes solution of the nonlinear state equation. This seems to be unsatisfactory from a practical point of view, where one would like to be able to do a single linearization step. By including the residual of the nonlinear equation into the estimator, it seems to possible to generalize the perturbed gradient method in this direction.

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