

# Theory for Boundary-Value Objective-First Optimization

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## 1 Improving the field

We begin by writing down a generic (sourceless) physics problem,

$$A(p)x = 0. \tag{1}$$

Here,  $x$  is the field variable,  $p$  is the structure variable, and  $A(p)$  represents the physics of the problem.

Now, suppose that we want to fix the value of the field at certain grid-points. We denote these fixed points as *boundary values* of the problem. Specifically, we break up  $x$  into

$$x = S_1x_1 + S_0x_0, \tag{2}$$

where  $S_1$  and  $S_0$  are selection matrices for the varying and fixed elements of  $x$  respectively.

We can now attempt to solve eq. 1 by finding  $x_1$  in the following manner. Let

$$A(p)S_1x_1 = -S_0x_0, \tag{3}$$

or

$$\hat{A}(p)x_1 = b, \tag{4}$$

where  $\hat{A}(p) = A(p)S_1$  and  $b = -S_0x_0$ .

Note that there often will not be a valid  $x_1$  to satisfy eq. [?] since  $\hat{A}(p)$  will in general be skinny and full-rank. Instead, we can minimize the *physics residual*, defined as

$$\|A(p)x\|^2 = \|\hat{A}(p)x_1 - b\|^2. \tag{5}$$

We call solving the problem

$$\underset{x_1}{\text{minimize}} \quad \|\hat{A}(p)x_1 - b\|^2 \quad (6)$$

improving the field. Note that an equivalent problem definition is

$$\underset{x}{\text{minimize}} \quad \|A(p)x\|^2 \quad (7)$$

$$\text{subject to} \quad S_0^T x = x_0. \quad (8)$$

## 2 Improving the structure

We now consider the structure improvement problem, that is,

$$\underset{p}{\text{minimize}} \quad \|A(p)x\|^2. \quad (9)$$

Whereas the field improvement problem can always be solved exactly, this is not the case for the structure improvement problem. Even when  $A(p)$  is linear with respect to  $p$ , there are often restrictions on  $p$  which make finding a solution very difficult. For example, a common restriction is that  $p$  be binary, that is,  $p \in \{0, 1\}$ . In this case, the problem is generally NP-hard. For these reasons, we often use a simple gradient-descent method to arrive at an approximate solution of eq. 9.

If  $A(p) = A_1 \text{diag}(A_2 p) A_3$  then,

$$A(p)x = A_1 \text{diag}(A_2 p) A_3 x \quad (10)$$

$$= A_1 \text{diag}(A_3 x) A_2 p \quad (11)$$

$$= B(x)p. \quad (12)$$

where  $B(x) = A_1 \text{diag}(A_3 x) A_2$ .

The gradient of the physics residual with respect to  $p$  can then be computed using

$$\frac{\partial}{\partial p} \frac{1}{2} \|A(p)x\|^2 = \frac{\partial}{\partial p} \frac{1}{2} \|B(x)p\|^2 = B(x)^* B(x)p. \quad (13)$$

## References