Boundary terms

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1 Variation of Boundary terms

1.1 Boundary integrals and Mayer-Bolza problem

A natural extension of the simplest variational problem is the Mayer-Bolza problem of minimization of the sum of the volume and the boundary integrals

$$I(u) = \min_u \left(\int_\Omega F(x, u, \nabla u) dx + \int_{\partial\Omega} f(s, u) ds \right) \tag{1}$$

This problem arises in physical applications when the boundary energy is taken into account, and in optimization theory where the functionals often have boundary terms.

The increment of the functional consists of the bulk and boundary parts:

$$\delta I = \int_\Omega S(x, u, \nabla u) \delta u \, dx + \int_{\partial\Omega} B(s, u, u_n) \delta u \, ds$$

The boundary integral does not contribute to the bulk part and to the Euler equation in Ω. It remains the same as is defined in (**??**) and the bulk part of stationarity condition remains

$$S_F(u) = \frac{\partial F}{\partial u} - \nabla \cdot \left(\frac{\partial F}{\partial \nabla u} \right) = 0.$$

The boundary term B consists of the term $\frac{\partial F}{\partial \nabla u} \cdot n \delta u$ that is supplied by the variation of the bulk integral (via integration by parts, compare with (**??**)), and $\frac{\partial f}{\partial u} \delta u$-term supplied by the variation of the boundary integral:

$$B(s, u, u_n) \delta u = \left(\frac{\partial F}{\partial \nabla u} \cdot n + \frac{\partial f}{\partial u} \right) \delta u$$

When no extra conditions are prescribed on the boundary, the stationary condition (natural boundary condition) holds:

$$B(s, u, u_n) = \frac{\partial F}{\partial \nabla u} \cdot n + \frac{\partial f}{\partial u} = 0 \quad \text{on } \partial\Omega, \quad \text{if } \delta u \text{ is arbitrary.} \tag{2}$$

Notice, that this condition degenerates into natural boundary condition (**??**) when the boundary term is zero, $f = 0$. In physical applications, the boundary integral often represents the work of external forces against the potential u. In this case, the force p equals $p = \frac{\partial f}{\partial u}$.

Next examples derive a variational problem corresponding to various classical types of boundary value problems for Laplace equation.

Variational origin of the Dirichlet, Neumann, and Robin problems Consider minimization of the functional:

$$I(u) = \min_u \left[\frac{1}{2} \int_\Omega |\nabla u|^2 dx + \int_{\partial\Omega} \left(\frac{1}{2} a(s) u^2 + b(s) u \right) ds \right]$$

for given functions $a(s), b(s)$. The Euler equation in the domain Ω is the Laplace equation:

$$\Delta u = 0 \quad \text{in } \Omega$$

The natural boundary condition is:

$$\frac{\partial u}{\partial n} + a(s)u + b(s) = 0 \quad \text{on } \partial\Omega$$

This is the so-called radiation condition (Robin condition) that specifies the rate of radiation $\frac{\partial u}{\partial n}$ depending on the value of u.

- When $a = b = 0$, the condition becomes homogeneous Neumann condition (an insulation condition);
- when $a = 0$ we deal with inhomogeneous Neumann conditions.
- To obtain inhomogeneous Dirichlet condition $u = \beta(s)$, we use the representation $b(s) = \beta(s)a(s)$ and consider the limiting case of the natural condition when $a(s) \to \infty$.

The work of external boundary force p against the potential u corresponds to the force $p = -a(s)u - b(s)$.

Problem 1.1 Determine the boundary term in the Mayer-Bolza problem which corresponds to the boundary Lagrangian (boundary energy) $f = \alpha u^3$, α is a scalar.

1.2 Examples

Inversion: Determination of the Lagrangian from Euler equation After the link between the variational problem and the boundary value problem is established, one can invert the situation and ask what variational functional corresponds to the given boundary value problem which we treat as the stationary condition to the unknown variational problem. Of course, we do not expect to obtain a unique solution. For instance, the null-Lagrangians cannot be accounted for. However, in many cases the variational problem can be easily guessed, as it is demonstrated at the next example.

Example 1.1 (Radiation of the black body) Consider the following inverse variational problem. Find the variational principle for the absolutely black body Ω with the radiation law ()

$$\frac{\partial \theta}{\partial n} = \gamma \theta^4 \quad \text{on } \partial\Omega$$

where is the absolute (*Kelvin* temperature; temperature θ is harmonic inside the body.

Using the previous paragraph, we easily guess the bulk and boundary terms in the Lagrangian

$$\min_{\theta} I(\theta), \quad I(\theta) = \left[\int_{\Omega} \frac{1}{2} (\nabla \theta)^2 dx + \frac{\gamma}{5} \int_{\partial\Omega} \theta^5 ds \right]$$

and thus formulate the variational principle of the radiative absolutely black body that obeys Stefan – Boltzmann law.

Example 1.2 (Relaxed harmonic continuation) Let us return to the problem of funding a harmonic extension to a boundary term, see Example **??**. Now we relax the problem's condition: Instead of prescribing the boundary data $u|_{\partial\Omega} = \phi(s)$ at every boundary point, we penalize solution for its deviation from the prescribed boundary value $\phi(s)$. Assuming that the penalty is proportional to the square of L^2 norm of the difference, we formulate the problem of *relaxed harmonic extension*:

$$\min_u I, \quad I = \int_\Omega |\nabla u|^2 dx + \beta \int_{\partial\Omega} (u-\phi)^2 ds$$

where $\beta > 0$ is the penalization parameter. The stationarity conditions are

$$\Delta u = 0 \ \text{ in } \Omega, \quad \frac{1}{\beta}\frac{\partial u}{\partial n} + u = \phi \ \text{ on } \partial\Omega \tag{3}$$

Minimizer u satisfies Laplace equation with the boundary conditions of the third type, which is the Robin problem. Notice that the minimizer tends to the minimizer of the problem in Example **??** if $\beta \to \infty$.

The solution allows for the following physical visualization. Imagine that u is the temperature. The problem in Example **??** describes the temperature distribution in a body with the fixed boundary temperature. The relaxed problem describes the temperature distribution in a body with the radiation from /absorbtion at the boundary. The rate of radiation is proportional to the difference $(u - \phi)$ between the fixed boundary temperature and target function.

Example 1.3 (Relaxed harmonic extension in circular domain) Consider the harmonic extension in a circular domain $0 \le r \le 1$, $-\pi < \theta \le \pi$. Let expand the given on the boundary function $\phi(\theta)$ into Fourier series

$$\phi(\theta) = a_0 + \sum_{k=1}^{\infty} a_k \cos(k\theta)$$

where

$$a_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} \phi(\theta) d\theta, \quad a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} \phi(\theta)\cos(k\theta) d\theta.$$

are the known Fourier coefficients. The general solution of the Laplace equation in the circle has the form

$$u(r,\theta) = c_0 + \sum_{k=1}^{\infty} c_k r^k \cos(k\theta),$$

the coefficients c_k are found from the boundary condition in (3) as

$$c_0 = a_0, \quad \frac{k}{\beta}c_k + c_k = a_k$$

The solution to the relaxed continuation problem becomes

$$u(r, \theta) = a_0 + \sum_{k=1}^{\infty} \frac{\beta}{\beta + k} a_k \, r^k \, \cos(k\theta).$$

One observes that the coefficients by high harmonics ($k \gg 1$) in $u(r, \theta)$ are dumped due to relaxation. In other words, the problem of relaxed extension is the extension problem of (Example ??) with smoothed boundary data ϕ_{smooth} instead of ϕ. This smoothed data are given by the Fourier series

$$\phi_{\mathrm{smooth}}(\theta) = a_0 + \sum_{k=1}^{\infty} \frac{\beta}{\beta + k} a_k \, r^k \, \cos(k\theta).$$

The solution to the stationary problem may not exist We remind that the stationarity is the necessary condition of the extremum. If the minimizer to the variational problem is continuous and differentiable, then it satisfies the stationary conditions. Next example shows that the Mayer-Bolza problem may lead to contradictory requirements so that the stationary solution of the problem does not exist.

Example 1.4 (Controversial boundary conditions) Consider the problem

$$I(u) = \min_u \int_\Omega |\nabla u| dx + \int_{\partial\Omega} a u \, ds$$

or $F = |\nabla u|, \quad f = au$. The Euler equation in Ω was derived in the previous section, example ??. The boundary condition is

$$\frac{\nabla u \cdot n}{|\nabla u|} + a = 0$$

The first term in the left-hand side of the last expression is equal to the cosine of the angle between the normal n and the direction $\frac{\nabla u}{|\nabla u|}$ of the gradient; therefore the boundary condition becomes

$$\cos(\widehat{n, \nabla u}) = -a$$

The last condition is not controversial if $|a| \leq 1$ everywhere on $\partial\Omega$. If $|a| = 1$, the direction of gradient coincide with the normal n, if $a = 0$, $\nabla u \cdot n = 0$. However, if $|a(s)| \geq 1$ for some s on $\partial\Omega$, solution to the boundary values problem does not exists. We conjecture that the true minimizer is discontinuous and does not corresponds to the Euler equation.

1.3 Weierstrass-Erdman condition for discontinuous Lagrangians

Discontinuity in the coefficients of the Lagrangian results in the Weierstrass-Erdman condition which should be satisfied on a surface where the gradient of the extremal is discontinuous. Assume that a two-dimensional domain Ω is divided into two connected subdomains Ω_1 and Ω_2 with the common boundary component ∂_{12} and that the boundary is assumed is a twice differentiable surface; Lagrangian F is defined by two different expressions in Ω_1 and Ω_2

$$F(x, u, \nabla u) = \begin{cases} F_1(x, u, \nabla u) & \text{if } x \in \Omega_1 \\ F_2(x, u, \nabla u) & \text{if } x \in \Omega_2 \end{cases} .$$

Consider the variational problem with the objective functional I,

$$I = \int_\Omega F(x, u, \nabla u) dx = \int_{\Omega_1} F_1(x, u, \nabla u) dx + \int_{\Omega_2} F_2(x, u, \nabla u) dx \tag{4}$$

over $u(x)$. The Weierstrass-Erdman condition is the boundary condition on the shared part ∂_{12} of the boundary. On this surface, two conditions on u and $\frac{\partial u}{\partial n}$ are needed to uniquely continue the solution from one subdomain to the other.

First condition The first (main) condition is the requirement of continuity of potential u. It is differentiable everywhere in Ω, including boundary ∂_{12}, therefore

$$[u]_2^1 = 0 \tag{5}$$

where $[]_2^1$ denotes the jump at $\partial\Omega$,

$$[u]_2^1 = u(x + \epsilon_1) - u(x + \epsilon_2), \quad x \in \partial_{12},\ x + \epsilon_i \in \Omega_i,\ |\epsilon_i| \to 0\ , i = 1, 2$$

This condition implies the continuity of the tangential derivative $\frac{\partial u}{\partial t}$ where t is a tangent to ∂_{12}.

$$\left[\frac{\partial u}{\partial t} \right]_2^1 = 0 \quad \text{on } \partial_{12} \tag{6}$$

Indeed, consider two pairs of point x_{1a}, x_{2a} and x_{1b}, x_{2b} lying on opposite sides of ∂_{12}, $x_{1a}, x_{1b} \in \Omega_1$ and $x_{2a}, x_{2b} \in \Omega_2$ such that the distances between the points on the opposite sides of the boundary is much smaller than distance between points on the same side:

$$\|x_{1a} - x_{1b}\| = \epsilon,\ \|x_{2a} - x_{2b}\| = \epsilon,\ \|x_{1a} - x_{2a}\| = \delta\epsilon,\ \|x_{1b} - x_{2b}\| = \delta\epsilon,$$

where $\epsilon \ll 1, \delta \ll 1$ are positive parameters. Notice that the direction of vectors $x_{1a} - x_{1b}$ and $x_{2a} - x_{2b}$ tends to the tangent t of ∂_{12} at the point x, when $\epsilon \to 0,\ \delta \to 0$.

$$\lim_{\epsilon \to 0,\ \delta \to 0} \frac{x_{1a} - x_{1b}}{\|x_{1a} - x_{1b}\|} = t, \qquad \lim_{\epsilon \to 0,\ \delta \to 0} \frac{x_{2a} - x_{2b}}{\|x_{2a} - x_{2b}\|} = t.$$

Compute the potential at these points and assume that u is differentiable:

$$|u(x + \delta) - u(x)| \le A|\delta|, \quad \forall \delta, \forall x$$

Then the differences

$$Df_1 := \frac{u(x_{1a}) - u(x_{1b})}{\epsilon}, \quad Df_2 = \frac{u(x_{2a}) - u(x_{2b})}{\epsilon}$$

will differ by an order of δ:

$$|Df_1 - Df_2| \leq 2A\delta$$

The limits of Df_1 and Df_2, as $\epsilon \to 0$, tend to the tangent derivatives on both sides of ∂_{12},

$$\lim_{\epsilon \to 0} Df_1 = \frac{\partial u(x)}{\partial t}_1, \quad \lim_{\epsilon \to 0} Df_2 = \frac{\partial u(x)}{\partial t}_2.$$

and the difference between them tends to zero, when $\delta \to 0$. We arrive at the condition (6).

Remark 1.1 Notice that the condition is derived from the assumptions about smoothness of the solution and of the boundary.

Remark 1.2 In a three-dimensional problem, there are two independent tangential partial derivatives on the boundary in two orthogonal tangential directions. The both derivatives are continuous, if the potential is continuous.

Second condition The second (variational) condition is called the Weierstrass-Erdman condition. It comes from the first variation of the objective functional (4)

$$\begin{aligned} \delta I = & \int_{\Omega_1} S_{F_1}(u)\delta u\, dx + \int_{\Omega_2} S_{F_2}(u)\delta u\, dx \\ & + \int_{\partial\Omega_1} \frac{\partial F_1}{\partial \nabla u} n_1\, \delta u\, ds + \int_{\partial\Omega_2} \frac{\partial F_2}{\partial \nabla u} n_2\, \delta u\, ds \end{aligned}$$

where $S_{F_1}(u)$ and $S_{F_2}(u)$ are the terms in the Euler-Lagrange equations in the corresponding subdomains. The condition of stationarity of the integrals over Ω_1 and Ω_2 gives the Euler equations in these domains, and the boundary integrals give the variational boundary conditions. The variational condition on the shared boundary ∂_{12} involves both boundary integrals because the variation of δu is the same in both integrals, and the normals have opposite directions, $n_1 = -n_2$. (Different signs of the normal correspond to the agreement that the normal is outer-pointing with respect to the domain of variation. The outer normal to Ω_1 is the inner normal to Ω_2.) On the shared boundary ∂_{12}, we write the stationarity condition

$$\delta u : \int_{\partial_{12}} \left(\frac{\partial F_1}{\partial \nabla u} - \frac{\partial F_2}{\partial \nabla u} \right) \cdot n\, \delta u\, ds = 0$$

which leads to the Weierstrass-Erdman condition

$$\left. \frac{\partial F}{\partial \nabla u} \cdot n \right|_{-}^{+} = 0 \quad \text{on } \partial_{12}. \tag{7}$$

This condition is the direct analog of the Weierstrass-Erdman condition on the broken extremal in one-variable case (see Section **??**) which has the form $[\frac{\partial F}{\partial u'}]_-^+ = 0$. In multivariate case, the Weierstrass-Erdman condition depends on the normal to the surface (line) of the discontinuity. Hence the normal derivative of the minimizer can be discontinuous but instead the Weierstrass-Erdman condition holds. Simultaneously, the tangent derivative of the minimizer u remains continuous to preserve continuity of u at the common part of the boundary.

Example 1.5 (Inhomogeneous conducting medium) The steady state equation for a conducting medium corresponds to the variational problem with the Lagrangian $F = \frac{\kappa}{2}|\nabla u|^2$, where $\kappa = \kappa(x)$ is the conductivity. Assume that the medium is heterogeneous, and $\kappa(x)$ is a discontinuous function that takes two values κ_1 and κ_2 in Ω_1 and Ω_2, respectively,

$$\kappa(x) = \kappa_1\chi(x) + \kappa_2(1 - \chi(x)) \tag{8}$$

where

$$\chi(x) = \begin{cases} 1 & \text{if } x \in \Omega_1 \\ 0 & \text{if } x \notin \Omega_1 \end{cases} \tag{9}$$

Let us establish continuity conditions on the boundary ∂_{12} between Ω_1 and Ω_2. We set $F_i = \frac{\kappa_i}{2}|\nabla u|^2$, $i = 1, 2$ and compute $\frac{\partial F}{\partial \nabla u} \cdot n = \kappa \frac{\partial u}{\partial n}$. The continuity conditions (6), (7) on the boundary ∂_{12} become

$$\nabla u \cdot t|_2^1 = 0, \quad \kappa \nabla u \cdot n|_2^1 = 0,$$

or, in coordinates,

$$\frac{\partial u_2}{\partial t} = \frac{\partial u_1}{\partial t}, \quad \kappa_2 \frac{\partial u_2}{\partial n} = \kappa_1 \frac{\partial u_1}{\partial n} \quad \text{on} \quad \partial_{12}$$

where u_1 and u_2 are the minimizers in Ω_1 and Ω_2, respectively. These conditions allow for the following physical interpretation: the tangent component of the field $\nabla u \cdot t$ and the normal component of the current $j \cdot n = \kappa \nabla u \cdot n$ are continuous on the boundary between the domains of different conductivity.

1.4 Effective conductivity of a laminate

The derived formulas allow us to calculate the *effective conductivity* of a laminate composite. Consider a periodic laminate put into a homogeneous field V. Let Ω be a unit square $\Omega = [0, 1] \times [0, 1]$ divided into $\Omega_1 = [0, 1] \times [0, m]$ and $\Omega_2 = [0, 1] \times [m, 1]$. Denote the components of the boundary as $\partial_1, \ldots, \partial_4$

$$\partial_1 = \{x : \quad x_1 = 0, \quad x_2 \in [0, 1]\}, \quad \partial_2 = \{x : \quad x_1 = 1, \quad x_2 \in [0, 1]\},$$
$$\partial_3 = \{x : \quad x_1 \in [0, 1], \quad x_2 = 0\}, \quad \partial_4 = \{x : \quad x_1 \in [0, 1], \quad x_2 = 1\}.$$

The conductivity problem is subject to the boundary conditions $u|_{\partial_k} - u|_{\partial_{k-1}} = V$ for all k and one pair of boundary componentsand homogeneous Neumann conditions (insulation) on the rest of the boundary. This problem is a solution to the variational problem of minimization of the energy $W(\nabla u)$

$$W = \min_u \frac{1}{2} \int_\Omega \kappa |\nabla u|^2 dx, \quad \kappa(x) = \kappa_1 \chi(x) + \kappa_2 (1 - \chi(x)) \tag{10}$$

where χ is defined in (9) and the minimizer saisfies the corresponding conditions.

Consider the problem of the effective conductivity of the structure. To define the effective conductivity k_* we replace inhomogeneous conductivity in Ω with a new equivalent homogeneous material. Our goal is to express the energy as a quadratic form

$$W = \frac{1}{2} \nabla u_* \cdot \boldsymbol{\kappa}_* \nabla u_*, \quad \nabla u_* = \int_\Omega \nabla u \, dx$$

so that W be a function of the average gradient ∇u_*, where u is the solution of (10). This will determine the effective property κ_*. There are two cases that should be considered separately.

Case A. Let the field be applied along the layers. This is modeled by the main boundary conditions:

$$u = 0 \quad \text{if } x \in \partial_1, \quad u = V \quad \text{if } x \in \partial_2.$$

Notice that V is the intensity of the average field in the unit square domain, $V = |\nabla u_*|$. The stationary condition in the domains Ω_i and the natural condition $\nabla u \cdot n = 0$ on the horizontal boundaries ∂_3 and ∂_4 have the form

$$\kappa_i \Delta u = 0 \ \text{ in } \Omega_i, \quad i = 1, 2, \quad \frac{\partial u}{\partial x_2} = 0 \text{ on } \partial_3 \text{ and } \partial_4$$

They are satisfied if the potential u is a linear function of x_1:

$$u(x_1, x_2) = V x_1 \quad \text{in } \Omega_1 \text{ and } \Omega_2$$

The Weierstrass-Erdman condition is trivially satisfied because the field ∇u is parallel to the layers everywhere and $\frac{\partial u}{\partial n} = 0$. The energy W_A in this case is

$$W_A = \frac{1}{2} \int_\Omega \left(\kappa_1 |\nabla u|^2 \chi(x) + \kappa_2 |\nabla u|^2 (1 - \chi(x)) \right) dx = \frac{1}{2} \kappa_A V^2$$

where

$$\kappa_A = m\kappa_1 + (1 - m)\kappa_2$$

is the (arithmetic) effective conductivity of the laminate for the field applied along the layers.

Case B. Let the field be applied across the layers. The main boundary conditions are

$$u = 0 \quad \text{if} \quad x \in \partial_3, \quad \text{and} \quad u = V \quad \text{if} \quad x \in \partial_4,$$

where V is the intensity of the average field, $|\nabla u_*| = V$. The stationary conditions are:

$$\kappa_i \nabla^2 u = 0 \ \text{ in } \Omega_i, \quad i = 1, 2, \quad \frac{\partial u}{\partial x_1} = 0 \text{ on } \partial_1 \text{ and } \partial_2$$

They are satisfied if the potential is a continuous piece-wise linear function of x_2:

$$u(x_1, x_2) = \begin{cases} A_1 x_2 & \text{if } x_2 \in [0, m] \\ A_1 m + A_2(x_2 - m) & \text{if } x_2 \in [m, 1] \end{cases} \tag{11}$$

where A_1 and A_2 are chosen to satisfy the boundary condition

$$u(1) = A_1 m + A_2(1 - m) = V.$$

The second condition for the constants A_1 and A_2 follows from the Weierstrass-Erdman condition (7) on the boundary between Ω_1 and Ω_2:

$$\kappa \frac{\partial u}{\partial x_2}\bigg|_-^+ = \kappa_2 A_2 - \kappa_1 A_1 = 0$$

We find

$$A_1 = \frac{\kappa_2}{m\kappa_2 + (1 - m)\kappa_1} V, \quad A_2 = \frac{\kappa_1}{m\kappa_2 + (1 - m)\kappa_1} V$$

Substituting the found values of A_1 and A_2 into (11) and computing the energy, we have:

$$W_B = \frac{1}{2} \int_\Omega \left(\kappa_1 |\nabla u|^2 \chi(x) + \kappa_2 |\nabla u|^2 (1 - \chi(x)) \right) dx = \frac{1}{2} \kappa_H V^2$$

where κ_H

$$\kappa_H = \kappa_1 A_1^2 m_1 + \kappa_2 A_2^2 m_2 = \left(\frac{m}{\kappa_1} + \frac{1 - m}{\kappa_2} \right)^{-1}$$

is the (harmonic mean) effective conductivity of the laminate across the layers.

The results for the two different directions of the applied field are different from each other. This shows that the effective conductivity κ_* is anisotropic. The anisotropy is caused by the Weierstrass-Erdman condition which introduces the dependence on the normal to the boundary dividing the subdomains of different conductivity. One can show that effective conductivity is described by a symmetric tensor

$$\kappa_* = \begin{pmatrix} \kappa_A & 0 \\ 0 & \kappa_H \end{pmatrix}$$

with eigenvalues κ_A and κ_H.