SJÄLVSTÄNDIGA ARBETEN I MATEMATIK

MATEMATISKA INSTITUTIONEN, STOCKHOLMS UNIVERSITET

Calculus of variations and optimal control theory applied to material fracture

av

Jenny Carlsson

2019 - No K10

Calculus of variations and optimal control theory applied to material fracture

Jenny Carlsson

Abstract

Many naturally occurring processes follow some principle of optimality, e.g. the principle of minimisation of potential energy. As a consequence, optimisation provides invaluable tools in physics and engineering. Here, models for fracture of materials are investigated using calculus of variations and optimal control theory.

Three different models for predicting when (or if) fracture occurs are presented and investigated: Griffith's model, the variational approach to fracture and a set of models referred to as gradient regularised fracture models. They are all based on the principle of minimisation of potential energy, given an extended notion of potential energy as consisting of the sum of the elastic energy and the surface energy of the (eventual) fracture surface.

The specific problem under consideration is that of uniaxial fracture of a rod subjected to a prescribed displacement in one end while the other end remains fixed. It is investigated in terms of solutions to the fracture problem given by the three different models, with emphasis on the gradient regularised models. Necessary conditions for the existence of minimisers are derived using both Euler-Lagrange equations and Pontryagin's minimum principle. Sufficient conditions for the existence of minimisers are investigated using the second variation. The essay also includes an introduction to calculus of variations and the related topic of optimal control theory.

i

Contents

iv

1 Introduction

Mathematical modelling is as integral to science and engineering as experimental observations are. Sometimes unknowingly, the scientist or engineer applies results from advanced topics of mathematics to predict e.g. physical phenomena. One such topic is that of optimisation. The underlying idea is beautiful; that naturally occurring processes are – in some sense – always optimal. Very often, this means optimal in terms of energy distribution and consumption. If natural states are optimal (as this is mostly unproven), then the large toolbox of e.g. calculus, calculus of variations and optimal control theory provides powerful tools to predict these states.

Calculus of variations originated with a question posed by Johann Bernoulli in 1696: which is the fastest path between two set points in a gravitational field? Several of the brightest mathematical minds of the time, including Newton, Leibnitz and Bernoulli himself, managed to solve the problem, and in the process invented a new branch of mathematics, now known as calculus of variations. (Zhou (2017a)) Around two hundred years later, at the turn of the twentieth century, David Hilbert addressed the issue of "further development of the calculus of variation" as the twentythird of his 23 unsolved problems of mathematics (Hilbert (1902)). This spurred a great development of calculus of variations in the twentieth century; much of this later development is referred to as optimal control theory (van Brunt (2006)).

In this work, we will explore the subjects of calculus of variations and optimal control theory. The specific topic of this work, which serves as the working example throughout the text, is material failure under mechanical loads. The strength of a material determines if and how that material can be safely used in an engineering design. Materials can be loosely divided into two categories, ductile materials, meaning materials that break by losing stiffness, leading to large deformations (e.g. most metals), and brittle materials meaning materials that break by sudden fracture without prior loss of stiffness (e.g. glass, ceramics).

Ductile materials can be described as stress-hardening materials, meaning that if the load (stress) is increased, then that increase is matched by the capacity to carry that load (even if it occurs with large deformations). When these materials are modelled mathematically, the governing equations are well-posed with unique solution. Brittle fracture is mathematically complicated due to stress-softening: if – at some critical load – we increase the load, the load carrying capacity of the material suddenly drops when the material fractures. Brittle fracture is often difficult to predict, and its consequences are often severe. Therefore, material fracture is of great importance in many engineering applications.

The outline of the work is as follows. First, we are given a very brief introduction to solid mechanics, and the problem of a unidirectional tensile fracture test is outlined (Section 1.1). This example will follow us throughout the work and serve as an illustration of the models

1

and methods introduced. We are then presented with three different mathematical models for fracture, the model suggested by Griffith (1921), the variational approach to fracture presented by Francfort and Marigo (1998) and a gradient regularised damage model (cf. Marigo et al. (2016)). Solutions to the unidirectional tension test problem using these models require some prior knowledge of calculus of variations, which will be given in Section 3, before we move on to solve the problem using the Euler-Lagrange equation. We will also solve the problem using optimal control theory, more specifically Pontryagin's minimum principle, which is done in Section 4. Both the Euler-Lagrange equation and Pontryagin's minimum principle provide only necessary conditions the existence of a minimum. A sufficient condition is derived in section 5. In physics, a minimum of potential energy means that a solution is observable and stable, which is why the fulfilment of the sufficient condition is sometimes referred to as stability.

In this essay I have primarily relied on the works of Logan (2013) for the section on calculus of variations, and on Sontag (1998) and Zhou (2017b) for the section on optimal control theory. The section on the second variation and stability is based mostly on van Brunt (2006). The applied sections dealing with the gradient regularised model of fracture are based primarily on Marigo et al. (2016); Pham et al. (2011).

1.1 The unidirectional tension problem

As a very simple model in a one-dimensional geometry, i.e. a rod, a solid material can be considered as a spring. When a spring with stiffness k is stretched a distance δ, it follows Hooke's law, i.e. the force F relates to the displacement as

$$F = k\delta. \tag{1}$$

A rod of cross-sectional area S, length L and material stiffness E will behave in the same way, with $k = ES/L$. It is often convenient to work with infinitesimal forces and displacements. Infinitesimal force is called stress, denoted σ. In one dimension $\sigma = F/S$. Infinitesimal displacement is dimensionless; it is called strain, denoted ε. Introducing the displacement at point x, i.e. $u(x) = \delta x/L$, we have

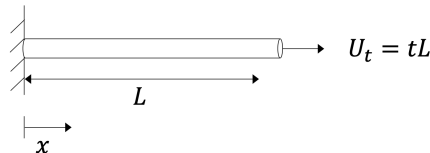$$\varepsilon(x) = u'(x) = \frac{\delta}{L}. \tag{2}$$

Figure 1: 1D tension problem with end displacement.

(Throughout, we will use prime notation to represent derivation with respect to x and a dot to represent derivation with respect to time t.)

In the following we will consider the case of a rod $\Omega = S \times [0, L]$, whose one end $(x = 0)$ is fastened to a rigid wall, while the other end $(x = L)$ is subjected to a prescribed, monotonically increasing, displacement $U_t = tL$, where t is time (Fig. 1). This deformation might seem extreme, but we can safely assume that $t = 1$ is large. (Having $U_t = tL$ instead of e.g. $U_t = \delta t$ where $\delta \neq L$ is some constant slightly simplifies later calculations.)

The rod has cross-sectional area S. The rod is made of a material with undamaged material stiffness E_0 and current (possibly reduced) material stiffness E. The displacement $u(x)$ of the bar is then

$$u(x) = tx.$$

Since the bar is one-dimensional, $u(x)$ only has one component, and the strain (i.e. gradient of $u(x)$) is scalar-valued,

$$\varepsilon(x) = u'(x) = t.$$

The stress of the rod is

$$\sigma(x) = E\varepsilon(x) = Et.$$

The strain energy density (the amount of strain energy stored in each infinitesimal element) of the rod is

$$E_d(x) = \frac{1}{2}\sigma(x)\varepsilon(x) = \frac{1}{2}Et^2,$$

giving the total strain energy in the body as

$$W_d(U_t) = \int_\Omega E_d d\Omega = \frac{1}{2}SLEt^2. \qquad (3)$$

The loading applied to the rod is considered to be slow and no inertia effects are included. The 1D tension problem will be revisited in Sections 3.3, 4.5 and 5.2.

This is the only background knowledge of solid mechanics required to follow the rest of this text. Of course, in more realistic applications, two- and three-dimensional geometries are also common. Solving these problems typically require numerical treatment which are beyond the scope of this thesis. My own interest in this project stems from my graduate work as a student in solid mechanics, in which I use gradient regularised models in finite element simulations of fracture of materials and complex geometries. My ambition was to understand them mathematically at a deeper level, the product of which is this essay.

2 Mathematical models of brittle fracture

In this chapter we are introduced to three different mathematical models of brittle fracture, which are the main topic of, as well as the working examples in, this work.

2.1 Griffith's model

The history of mathematical models of brittle fracture typically begins with Griffith (1921). Griffith was studying fracture in glass and found that there is no net change in energy during crack propagation. Assume the body in consideration is a subset of $\mathbb{R}^n$. Let $W_d : \mathbb{R}^n \to \mathbb{R}$ be the potential energy in the material, stored in the form of strain energy, and $W_s : \mathbb{R} \to \mathbb{R}$ be the surface energy of the crack. Then Griffith stated that

$$\frac{d(W_d + W_s - \mathcal{F})}{da} = 0, \tag{4}$$

i.e. as the crack advances a distance $da \in \mathbb{R}$, the change in energy given by the terms in the parenthesis is zero. The quantity $t \to \mathcal{F} : [0, \infty) \to \mathbb{R}$ is work by applied forces and $t \to a : [0, \infty) \to \mathbb{R}$ is the position of the crack tip. Further, he argued that a criterion for crack propagation is that

$$\frac{d(W_d - W_s)}{da} = 0, \tag{5}$$

a conclusion which probably requires some explanation. The surface energy, W_s, can be written as $W_s = \int_\Gamma G_c d\Gamma$, with Γ being the fracture surface and G_c the fracture toughness, or energy release rate. If $W_d \leq \int_\Gamma G_c d\Gamma$ then the derivative of the difference is nonzero, and crack propagation cannot occur. Further loading will increase W_d until the derivative becomes zero and crack propagation occurs by a distance determined by Eq. (5).

The derivative in (4) is equal to zero, which means that the energy in the numerator (possibly) has an extremum with respect to crack tip position. Griffith (1921) concluded that "The 'Theorem of minimum potential energy' may be extended so as to be capable of predicting the breaking loads of elastic solids, if account is taken of the increase in surface energy which occurs during the formation of cracks." In this spirit, we take account for the surface energy, and write W for potential energy in this sense, i.e. $W = W_d + W_s$.

The Griffith fracture model is revisited in Section 3.3.1.

2.2 The variational approach to fracture

Griffith's model was reformulated as a variational problem by Francfort and Marigo (1998). Griffith's model, while useful in predicting crack propagation, has some drawbacks. These drawbacks include that a crack will never initiate – unless there is already a crack there will never be failure. A second drawback is that of crack kinematics. In a

body $\Omega \subset \mathbb{R}^n$, a crack $\Gamma \subset \Omega$ is a closed subset of the body. A crack will typically have a dimension of $n-1$. This means that a crack can be parametrised by $n-1$ parameters, but require n functions of this/these parameter/s. However, Griffith's equations are scalar-valued, and the system is thus under-determined for $n > 1$.

In response to these drawbacks, Francfort and Marigo (1998) developed the variational approach to fracture, which hinges heavily on the works of Griffith, but resolves all of these drawbacks. They do this by considering a family of possible crack paths, each equipped with a (scalar) cost, i.e. an energy. For each member of the family of admissible displacement fields there is an associated energy, $W : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$, depending on the (time-dependent) displacement $t \to U(t) : [0, \infty) \to \mathbb{R}^n$ and (time-dependent) crack $t \to \Gamma : [0, \infty) \to \mathbb{R}^n$, defined as

$$W(\Gamma(t), U(t)) = W_d(\Gamma(t), U(t)) + W_s(\Gamma(t)), \tag{6}$$

with $W_d : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$

$$W_d(\Gamma(t), U(t)) = \int_\Omega E_d(\Gamma(t), U(t)) d\Omega$$

and $W_s : \mathbb{R} \to \mathbb{R}$

$$W_s(\Gamma(t)) = \int_{\Gamma(t)} G_c d\Gamma.$$

The evolution of the crack and energy follow three conditions:

(i) $\Gamma(t)$ is strictly increasing,

(ii) $W(\Gamma(t), U(t)) \leq W(\Gamma, U(t))$ for all $\Gamma \supset \cup_{s<t}\Gamma(s)$,

(iii) $W(\Gamma(t), U(t)) \leq W(\Gamma(s), U(t))$ for all $s < t$.

Conditions (i) and (ii) ensure that broken material does not heal, by requiring that the crack surface is non-decreasing and the previous cracks are enclosed in the current crack. Condition (ii) also ensures that the "real" crack is a minimum with respect to the cost/energy. The condition (iii) originates from the nature of the energies, $W_s(\Gamma(t))$ is strictly monotonically increasing in $\Gamma(t)$ and $W_d(\Gamma(t), U(t))$ is decreasing (but not strictly) for any fixed $U(t)$.

The crack state is found as the infimum of (6), as will be treated in Section 3.3.2. But, as will be illustrated briefly in the next section, this infimum is generally not trivial to find, which is the reason we now introduce the topic of gradient regularised damage models.

2.3 Gradient regularised damage models

Analytical and numerical implementation was considered a drawback of the variational approach to fracture, also by the authors themselves (Francfort and Marigo (1998)). But they also suggested what would turn out to be a very efficient workaround – the remarkable similarity between the variational fracture functional and the Mumford-Shah functional used for for image segmentation! Thus, the first numerical

experiments in the variational approach to fracture used this similarity to apply the already known Ambrosio-Tortorelli functional approximating the Mumford-Shah functional.

Ductile materials can be modelled using so-called damage models (standard damage models). In standard damage models, an internal variable is introduced; this variable represents the degree of damage in a region of the material based on the load. The damage variable typically determines the degree of stiffness loss. Since the material is stress-hardening, it keeps its load-carrying capacity even when damaged and damage does not localise into a crack. Brittle materials, on the other hand, can typically not be modelled using standard damage models. For strain-softening materials, damage tends to localise in a narrow band of zero thickness. But since this crack will have zero measure no energy is dissipated, which violates Griffith's Eq. (4).

To overcome this drawback, some regularisation of the damage is needed. A possible choice – stemming from the Ambrosio-Tortorelli functional – is to regularise the damage field by the gradient of the damage variable, thus dividing the surface energy into two terms, one local and one non-local (gradient-dependent). Models of this kind are called gradient damage models. The rest of this section is based on Marigo et al. (2016).

We consider again an n-dimensional body occupying the set $\Omega \subset \mathbb{R}^n$. Assume the body is made of a brittle material. Let $t \to d : [0, \infty) \to [0, 1]$ be a scalar damage variable, and let $d = 0$ represent intact material and $d = 1$ fully broken material. A prototype gradient damage model, depending on the displacement $t \to U, [0, \infty) \to \mathbb{R}^n$ and damage d, is then given by the energies $W_s : [0, 1] \to \mathbb{R}$, $W_d : \mathbb{R}^n \times [0, 1] \to \mathbb{R}$

$$W_s(d(t)) = \int_\Omega w(d(t)) + \frac{1}{2}w_1 l^2 (\nabla d(t))^2 d\Omega,$$

and

$$W_d(U(t), d(t)) = \int_\Omega E_d(U(t), d(t)) d\Omega,$$

where $w_1 \in \mathbb{R}$ is a constant, $d \to w, [0, 1] \to [0, w_1]$ is a function describing the local dissipated energy during damage evolution and $l \in \mathbb{R}$ is a regularisation length called the characteristic internal length.

The evolution of damage must follow certain conditions, basically the same conditions as Subsection 2.2 (i) – (iii). Specifically, damage must be irreversible; since materials do not heal, damage can only grow. Also, the "real" state of the damage must be a minimum of the functional, thus any small variation $v \in \mathbb{R}^n$, $\beta \in [0, 1]$ of the minimiser (U_t, d_t) must give a greater energy. Lastly, due to physics, the energy balance must always hold:

(i) $\dot{d} \geq 0$,

(ii) $W(U_t + \epsilon(v - U_t), d_t + \epsilon(\beta - d_t)) \geq W(U_t, d_t) \forall \epsilon$ small,

(iii) $W(U_t, d_t) = \int_0^t \int_\Omega (E_d(t) - \mathcal{F}(t)) \, d\boldsymbol{x} dt.$

6

Gradient damage models and their solutions are revisited in Subsections 3.3.3, 3.3.4, 4.5 and 5.2.

3 Calculus of variations

Calculus of variations is the mathematical topic concerned with optimisation of variable quantities called functionals.

The material in this section is primarily adapted from Logan (2013).

3.1 Functionals

The theory of functionals and calculus of variations is perhaps best introduced by an analogy to calculus. In calculus, a central problem is to find extremals of functions.

Definition 3.1 (Function). *Let $X \subseteq \mathbb{R}$. A function is a rule*

$$f : X \to \mathbb{R}$$

that assigns a real number $f(x)$ to each point $x \in X$ of the domain X of f. The set $\{f(x) | x \in X\}$ is called the image of f.

If f is a function defined on an open interval I, then f has a local minimum at a point x_0 in I if $f(x_0) \leq f(x)$ for all x, satisfying $|x - x_0| < \delta$ for some δ. If f has a local minimum, and if f is differentiable in I, then

$$f'(x_0) = 0.$$

In calculus of variations, functionals, rather than functions, are optimised.

Definition 3.2 (Functional). *Let $A \subseteq V$ where V is a normed linear vector space of functions. A functional is a rule*

$$J : A \to \mathbb{R}$$

that assigns a real number $J(y)$ to each function $y \in A$ of a set A of admissible functions.

An archetype for a functional is an integral: an integral with integration limits assigns a real number to a function. The set A must be a normed linear vector space. We can then define a functional analogue to a derivative of a function. This is known as the Gâteaux derivative or first variation of J. Let ϵ be small and let $v \in A$ be a variation of $y = y_0$. The Gâteaux derivative is then given by

$$\delta J(y_0, v) = \lim_{\epsilon \to 0} \frac{J(y_0 + \epsilon v) - J(y_0)}{\epsilon} = \frac{d}{d\epsilon} J(y_0 + \epsilon v)|_{\epsilon=0}.$$

if the limit exists. In the case that J depends on not only one but two functions, $J : A \times A \to \mathbb{R}$ with $J = J(y, u)$, the Gâteaux derivative is given by

$$\delta J((y_0, u_0)(h, k)) = \lim_{\epsilon \to 0} \frac{J((y_0 + \epsilon h)(u_0 + \epsilon k)) - J(y_0, u_0)}{\epsilon}$$

$$= \frac{d}{d\epsilon} J((y_0 + \epsilon h)(u_0 + \epsilon k))|_{\epsilon=0},$$

assuming $\epsilon h \in A, \epsilon k \in A$ and ϵ small, given that the limit exists.

Theorem 3.1 (Necessary condition for extremals of functionals)**.** *Let $J : A \to \mathbb{R}$ be a functional on $A \subseteq V$. If $y_0 \in A$ is a local minimiser for J, meaning that $J(y)$ has a minimum when $y = y_0$, then*

$$\delta J(y_0, v) = 0,$$

if the first variation exists.

Proof. Let $J : A \to \mathbb{R}$ be a functional on $A \subseteq V$, and let y_0 be a minimiser for J. Let v be a variation of y_0 such that $y_0 + \epsilon v$ is in A. Then we can define the function $\mathcal{J}(\epsilon)$,

$$\mathcal{J}(\epsilon) = J(y_0 + \epsilon v)$$

which has a local minimum at $\epsilon = 0$. Hence $\mathcal{J}'(0) = 0$, regardless of the choice of v, which completes the proof. $\square$

Remark 3.1. *Both the theorem and the proof hold also for functionals of two (or more) functions.*

When $\delta J(y_0, v) = 0$ (or $\delta J((y_0, u_0), (h, k)) = 0$) regardless of the variation v (or h, k), we will write $\delta J(y_0) = 0$ (or $\delta J(y_0, u_0) = 0$).

3.2 Euler-Lagrange equations

Assume that $J(y)$ is of the form $J(y) = \int_a^b L(x, y, y')dx$ with $L \in C^2[a,b] \times \mathbb{R}^2$ and $y \in C^2[a,b]$, i.e. both L and y are twice differentiable with smooth first and second derivatives on the interval $[a, b]$. We can also assume that the values of y are known at the end points of the interval. Assuming y is a local minimiser of J, then a small variation ϵv, with $\epsilon v \in C^2[a, b]$ and $v(a) = v(b) = 0$, from the initial $J(y)$ gives

$$J(y + \epsilon v) = \int_a^b L(x, y + \epsilon v, y' + \epsilon v')dx.$$

Therefore,

$$\frac{dJ}{d\epsilon}(y + \epsilon v) = \int_a^b \frac{\partial}{\partial \epsilon} L(x, y + \epsilon v, y' + \epsilon v')dx =$$

$$\int_a^b \left[\frac{\partial L}{\partial y}(x, y + \epsilon v, y' + \epsilon v')v + \frac{\partial L}{\partial y'}(x, y + \epsilon h, y' + \epsilon v')v' \right] dx,$$

and the first variation of J is

$$\delta J(y, v) = \frac{dJ}{d\epsilon}(y + \epsilon v)|_{\epsilon=0} = \int_a^b \left(\frac{\partial L}{\partial y}(x, y, y')v + \frac{\partial L}{\partial y'}(x, y, y')v' \right) dx.$$

We will soon prove that the so-called Euler-Lagrange equations are a necessary requirement for a function to be a minimum of the functional. First, we introduce an important lemma.

9

Lemma 3.1 (Fundamental lemma of calculus of variations)**.** *If $x \to$ $f : [a, b] \to \mathbb{R})$ is continuous on $[a, b]$ and if*

$$\int_a^b f(x)v(x) = 0$$

for every $v \in C^2[a, b]$ with $v(a) = v(b) = 0$, then $f(x) = 0$ for all $x \in [a, b]$.

Proof. The proof is by contradiction. Assume for some x_0 in (a, b) that $f(x) > 0$. Since $f(x)$ is continuous, then $f(x) > 0$ for $x \in (x_1, x_2)$ with $x_1 < x_0 < x_2$ and since $v(x)$ can be any twice differentiable function, we can choose

$$v(x) = \begin{cases} (x - x_1)^3 (x_2 - x)^3, & x_1 \le x \le x_2, \\ 0 & \text{otherwise.} \end{cases}$$

Note that $v(x)$, like $f(x)$, is positive for $x \in (x_1, x_2)$. Then

$$\int_a^b f(x)v(x)dx = \int_{x_1}^{x_2} f(x)(x - x_1)^3 (x_2 - x)^3 dx > 0,$$

so $f(x)$ cannot be positive for $x \in (a, b)$. If $f(x_0) < 0$ instead, we can choose v to be the negative of what we had above, which, like $f(x)$, would be negative for $x \in (x_1, x_2)$, and again we get a contradiction. So it must be that $f(x) = 0$. $\square$

Theorem 3.2 (Euler-Lagrange equations are a necessary condition for a local minimum)**.** *If a function y provides a local minimum of the functional $J(y) = \int_a^b L(x, y, y')dx$, where $L \in C^2[a, b] \times R^2, y \in C^2[a, b]$, and the values of y are known at the end points of the internal, then y must satisfy*

$$\frac{\partial L}{\partial y}(x, y, y') - \frac{d}{dx} \frac{\partial L}{\partial y'}(x, y, y') = 0, \quad x \in [a, b]. \tag{7}$$

Proof. As we saw earlier, a necessary condition for y to be a minimum is that

$$\int_a^b \left(\frac{\partial L}{\partial y}(x, y, y')v + \frac{\partial L}{\partial y'}(x, y, y')v' \right) dx = 0,$$

with $v(a) = v(b) = 0$. If we integrate the second term by parts, we obtain

$$\int_a^b \left(\frac{\partial L}{\partial y}(x, y, y') - \frac{d}{dx} \frac{\partial L}{\partial y'}(x, y, y') \right) vdx + \frac{\partial L}{\partial y'}(x, y, y')v|_{x=a}^{x=b} = 0. \tag{8}$$

Since $v(a) = v(b) = 0$ the last term is zero. Turning to the integral, since $v(a) = v(b) = 0$ then by the fundamental lemma of calculus of variations the expression in brackets must be equal to zero, which proves that the Euler-Lagrange equations are a necessary condition for y to be a minimiser of J. $\square$

10

Remark 3.2. *The condition that y is known at the end points (direct boundary conditions) restricts the admissible functions $h(x)$ to ones for which $v(a) = v(b) = 0$. If we do not know the value of, say $y(b)$, the last term of (8) is not (necessarily) zero and we would require a natural boundary condition $\partial L/\partial y'(b, y(b), y'(b)) = 0$ to determine the minimiser. The interested reader is referred to Logan (2013), p. 249ff.*

3.2.1 Euler-Lagrange equations with several dependent variables

The variational problem considered in the previous subsection, where J only depends on x, y and y', can be generalised in different ways. One way is to include higher order derivatives. This leads to a higher order ordinary differential equation of the form (see Logan (2013) for proof as it will not be used in our later derivations)

$$\frac{\partial L}{\partial y} - \frac{d}{dx}\frac{\partial L}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial L}{\partial y''} - ... + (-1)^n \frac{d^n}{dx^n}\frac{\partial L}{\partial y^{(n)}} = 0.$$

Another way is to let J depend on not only one function y and its first (or higher-order) derivative, but many functions $y_1, ..., y_n$ and their first (or higher-order) derivatives. In our case, the gradient enhanced model is a function of several variables u, d and their first derivatives.

Theorem 3.3 (Euler-Lagrange equations in several variables)**.** *If a function $y_1, ..., y_n$ provides a local minimum of the functional*

$$J(y_1, ...y_n) = \int_a^b L(x, y_1, ..., y_n, y', ..., y_n')dx,$$

where $y_1, ..., y_n \in C^2[a, b]$ with known boundary values at the endpoints, then $y_1, ..., y_n$ must satisfy

$$\frac{\partial L}{\partial y}(x, y_i, y_i') - \frac{d}{dx}\frac{\partial L}{\partial y_i'}(x, y_i, y_i') = 0, \quad i = 1, ..., n, \quad x \in [a, b]. \quad (9)$$

Proof. Assume $y_1, ..., y_n$ are the minimisers of J. Let $\epsilon v_1, ..., \epsilon v_n$, with ϵ small and $v_1, ..., v_n \in C^2[a, b]$, be a small variation, satisfying $v_1(a) = ... = v_n(a) = v_1(b) = ... = v_n(b) = 0$. Then the function

$$\mathcal{J}(\epsilon) = \int_a^b L(x, y_1 + \epsilon h_1, ..., y_n + \epsilon v_n)dx$$

has local minimum at $\epsilon = 0$. The derivative of $\mathcal{J}$ with respect to ϵ evaluated at $\epsilon = 0$ must be zero

$$\mathcal{J}'(0) = \int_a^b \left(\frac{\partial L}{\partial y_1}v_1 + ... + \frac{\partial L}{\partial y_n}v_n + \frac{\partial L}{\partial y_1'}v_1' + ... + \frac{\partial L}{\partial y_n'}v_n'\right) dx = 0.$$

Integrating the derivative terms by parts and using the fact that $v_1, ..., v_n$ are zero at the boundary points a, b gives

$$\mathcal{J}'(0) = \int_a^b \left[\left(\frac{\partial L}{\partial y_1} - \frac{d}{dx} \frac{\partial L}{\partial y_1'} \right) v_1 + \dots + \left(\frac{\partial L}{\partial y_n} - \frac{d}{dx} \frac{\partial L}{\partial y_n'} \right) v_n \right] dx = 0.$$

Since $v_1, \dots v_n$ can be any variation, say $v_i \neq 0$, $v_1 = \dots = v_{i-1} = v_{i+1} = v_n = 0$, we require that

$$\int_a^b \left(\frac{\partial L}{\partial y_i} - \frac{d}{dx} \frac{\partial L}{\partial y_i'} \right) v_i dx = 0$$

for each i, and the proof follows by the fundamental Lemma which says that the expression in parentheses must be zero.

$\square$

3.3 Application to the uniaxial tension test

Here we apply calculus of variations to the previously described models for fracture (cf. Section 2). The first two examples are not readily written as functionals of the form we require to apply e.g. the Euler-Lagrange equation. Due to this drawback, these models are rather limited in scope, whereas the latter models are have proved very versatile, especially when combined with numerical analysis.

3.3.1 Griffith's model

We now consider the uniaxial tension of the bar using Griffith's model. Consider the bar $\Omega = S \times [0, L]$ with cross sectional area S, subjected to end displacement $U(0) = 0$ and $U(L) = tL$ (Fig. 1).

Initially the bar is crack free, thus $W_s = 0$ and

$$W_d = \frac{1}{2} SLEt^2.$$

According to Griffith's theory, crack propagation requires that the criterion (4) is fulfilled, i.e. that

$$\frac{d(E_d + E_s)}{da} = \frac{d}{da} \left(\frac{1}{2} SLEt^2 + E_s \right) = 0 + \frac{dE_s}{da} = 0.$$

We see that regardless of the size of the loading tL the surface energy cannot change, thus, no crack will ever develop unless there is already a crack. We can also use the propagation criterion (5),

$$\frac{d(E_d - E_s)}{da} = \frac{d}{da} \left(\frac{1}{2} SLEt^2 \right) = 0.$$

Since E_d does not depend on a, this is always fulfilled, even without any loading.

Remark 3.3. *The derivative of (5) is of course always zero for no crack and no deformation, $E_s = 0$, $E_d = 0$. This is a trivial case since it also requires that, by (4), the external work is zero.*

3.3.2 The variational approach to fracture

We now turn to the uniaxial tension of the bar using the variational approach to fracture. This problem was first solved by Francfort and Marigo (1999). Consider the bar $\Omega = S \times [0, L]$, subjected to end displacement $U(0) = 0$ and $U(L) = tL$ (Fig. 1).

Initially, the bar is crack free (the crack $\Gamma = \O$, the empty set), thus $E_s = 0$ and

$$W(\O, U_t) = W_d(\Gamma, U_t) = S\frac{1}{2} \int_0^L \sigma\varepsilon dx = \frac{1}{2}SLEt^2.$$

After the rod is broken, $W_d = 0$ and

$$W(\Gamma, U_t) = W_s(\Gamma) = S\sum_{x \in \Gamma} G_c.$$

Let $W(\Gamma, U_t) = W_d(\Gamma, U_1) + W_s(\Gamma)$ be the functional that should be minimised. Since $W_d > 0$ implies $W_s = 0$ and $W_s > 0$ implies $W_d = 0$, and since W_d grows as t increases, $W(\Gamma, U_t)$ must be equal to W_d until $W_d = W_s$, after which the minimum of $W(\Gamma, U_t)$ is given by W_s. The equality occurs at

$$\frac{1}{2}SLEt^2 = SG_c.$$

Solving for tL gives the critical time t_c as

$$t_c = \sqrt{\frac{2G_cL}{E}}.$$

At this time $t = t_c$, the displacement of the rod is $u_c(x) = x\sqrt{2G_cL/E}$, the strain is $\varepsilon_c(x) = \sqrt{2G_cL/E}$ and the stress is $\sigma_c(x) = \sqrt{2EG_cL}$. The force response under continuous loading is thus linear with constant slope until t_c after which the force is zero (Fig. 2). The evolution and distribution of the total energy is plotted in Fig. 3.
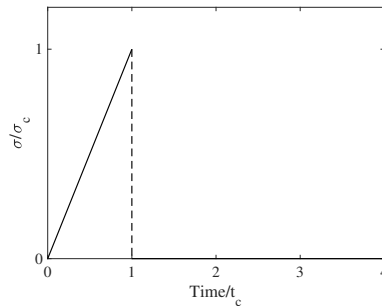

Figure 2: Normalised stress plotted versus normalised time (or normalised strain).
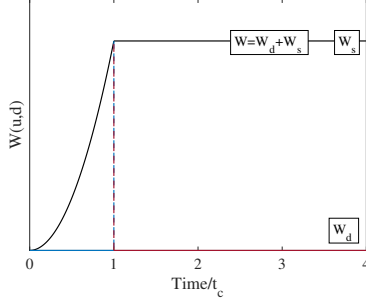
Figure 3: Total energy (black line) plotted against normalised time. The contributions from strain energy (red line) and surface energy (blue line) is also indicated.

3.3.3 Gradient regularised damage model with an elastic phase

We will now consider two different gradient regularised models in uniaxial tension. Consider again the bar $\Omega = S \times [0, L]$, subjected to end displacement $U(0) = 0$ and $U(L) = tL$ (Fig. 1). We introduce the new parameters $d(x)$, representing the damage, and l, the regularisation length, or width of the regularised crack. Since we have introduced the damage model (cf. Subsection 2.3) the energy related to the fracture surface is

$$W_s(u, d) = S \int_0^L \left(w(d) + \frac{1}{2} w_1 l^2 d'^2 \right) dx,$$

where we have dropped the ∇d notation in favour for d' since d only has derivative in x direction. We also have

$$W_d(u, d) = S \int_0^L \frac{1}{2} Et^2 dx = \frac{1}{2} SLEt^2.$$

The first model we consider is a damage model with choices $E = E_0(1 - d)^2$ and $w(d) = w_1 d$. The criterion Subsection 2.3 (ii) then translates into the following functional, which we want to minimise,

$$W(u, d) = S \int_0^L \left[w_1 d + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0(1 - d)^2 t^2 \right] dx. \qquad (10)$$

Unlike the previous examples, we are now able to use methods from calculus of variations. The functional in (10) has Lagrangian

$$\mathcal{L}(u, d) = w_1 d + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0(1 - d)^2 t^2.$$

The Euler-Lagrange equation (cf. 9) with respect to u (remembering that t^2 is actually u'^2) is

14

$$\frac{\partial \mathcal{L}}{\partial u} - \frac{d}{dx}\left(\frac{\partial \mathcal{L}}{\partial u'}\right) = -\frac{d}{dx}E_0(1-d)^2 u' = 0, \qquad (11)$$

which means that $\varepsilon' = u'' = 0$ i.e. that the strain must be constant, which we actually already knew. The Euler-Lagrange equation (9) of (10) with respect to d is

$$\frac{\partial \mathcal{L}}{\partial d} - \frac{d}{dx}\left(\frac{\partial \mathcal{L}}{\partial d'}\right) = w_1 - E_0(1-d)t^2 - w_1 l^2 d'' = 0. \qquad (12)$$

Rearranging the terms of (12) and observing that the second derivative of $d(x)$ must be zero (due to the geometry and load case we must have constant damage) we find that the Euler-Lagrange equation for d cannot be fulfilled until $t_c = \sqrt{w_1/E_0}$, or $U_c = L\sqrt{w_1/E_0}$. Thus the rod remains crack free with $d = 0$ with constant stiffness $E = E_0$ until $t = t_c$. At this time, the displacement of the rod is $u(x) = x\sqrt{w_1/E_0}$, the strain is $\varepsilon(x) = \sqrt{w_1/E_0}$ and the stress is $\sigma(x) = \sqrt{E_0 w_1}$.

After t_c, damage is evolving and the Euler-Lagrange equation is fulfilled, i.e.

$$w_1 = E_0(1-d)t^2.$$

which combined with the expression for t_c (and since damage cannot be negative) gives the damage as

$$d = \max\left(0, 1 - \left(\frac{t_c}{t}\right)^2\right),$$

and thus the also stress (Fig. 4),

$$\sigma = \begin{cases} \sigma_c \frac{t}{t_c} & \text{if } t \le t_c, \\ \sigma_c \left(\frac{t_c}{t}\right)^3 & \text{otherwise.} \end{cases} \qquad (13)$$

We see that the stress (or the load-carrying capacity of the rod) falls quickly and approaches zero (Fig. 4).
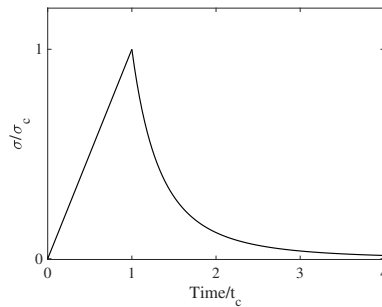

Figure 4: Normalised stress plotted versus normalised time (or normalised strain).

For completeness, we should also have a look at the energy, the functional whose value we are trying to minimise. The total energy depends on the displacement (or time) as (Fig. 5),

$$W(u, d) = \begin{cases} \frac{1}{2} SLE_0 t^2 & \text{if } t \leq t_c, \\ \frac{1}{2} SLE_0 \frac{t_c^4}{t^2} + SLE_0(t^2 - t_c^2) & \text{otherwise.} \end{cases}$$

Remark 3.4. *If we had not been able to make the assumption $d'' = 0$, we would have been forced to solve a partial differential equation (remember that $t = u'$), which can be done e.g. using numerical analysis. The assumption that $d'' = 0$ is only valid for the particular toy problem at hand.*

Figure 5: Total energy (black line) plotted against normalised time. The contributions from strain energy (red line) and surface energy (blue line) is also indicated.

3.3.4 Gradient regularised damage model without elastic phase

If we instead consider the model with the choices $E = E_0(1 - d)^2$ and $w(d) = w_1 d^2$, the criterion Subsection 2.3 (ii) translates into

$$W(u, d) = S \int_0^L \left[w_1 d^2 + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0(1 - d)^2 t^2 \right] dx. \qquad (14)$$

The Euler-Lagrange equations of (14) with respect to d is

$$\frac{\partial \mathcal{L}}{\partial d} - \frac{d}{dx} \left(\frac{\partial \mathcal{L}}{\partial d'} \right) = 2w_1 d - E_0(1 - d)t^2 - w_1 l^2 d'' = 0. \qquad (15)$$

If, as before, we solve for time we see that

$$t = \sqrt{\frac{2w_1 d}{E_0(1 - d)}},$$

so damage must evolve from $t = 0$, i.e. there is no elastic phase in which $d = 0$. Damage must evolve as

$$d = \frac{E_0 t^2}{2w_1 + E_0 t^2}. \qquad (16)$$

The stress however, is

$$\sigma = E_0 (1 - d)^2 \sqrt{\frac{2w_1 d}{E_0 (1 - d)}}.$$

The stress takes on a maximum when the derivative with respect to strain (i.e. time) is zero. Using Eq. (16) we see that this happens when $d = 1/4$, which means $\sigma = \sigma_m = 3\sqrt{3}/(8\sqrt{2})\sqrt{w_1 E_0}$ (Fig. 6). At this point, $t_M = \sqrt{2w_1/(3E_0)}$ and $U_M = \sqrt{2w_1/(3E_0)}L$. Unlike the previous model, the Euler-Lagrange equation is satisfied during the whole evolution. The evolution and distribution of the total energy is plotted in Fig. 7.

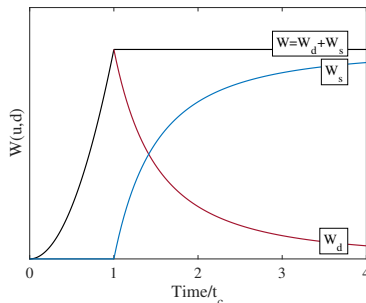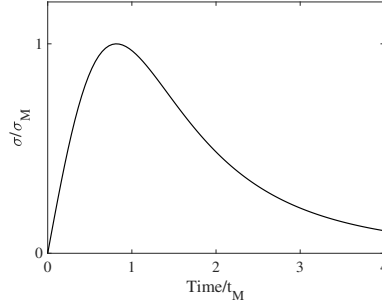Figure 6: Normalised stress plotted versus normalised time (or strain).
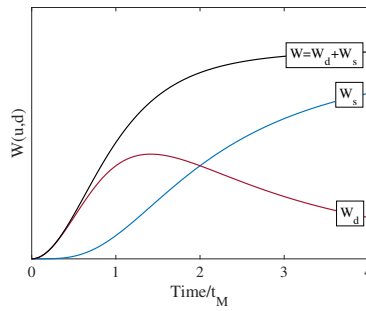

Figure 7: Total energy (black line) plotted against normalised time (or strain). The contributions from strain energy (red line) and surface energy (blue line) are also indicated.

4 Optimal control theory

Optimal control theory is, as the name suggests, related to control theory. Typical control problems include controlling the position of a robot arm, controlling the temperature inside a building, controlling the speed of a car when driving with cruise control etc. A typical control problem consists of something that we want to control x, and a control u. If we want to control the position x (possibly non-scalar) of a robotic arm, then our control might be some moment that we apply to the joint of the arm. Sometimes the objective is to control an object such that its behaviour is an optimum: it can be a spacecraft whose trajectory should be optimised to minimise travel time and/or fuel consumption. This is the domain of optimal control theory.

But optimal control theory is also an extension of calculus of variations, and can be used to solve variational problems. In the end of this chapter we will rewrite the mathematical models for fracture as optimal control problems, in which we use our control to minimise the potential energy. The material in the first part of this chapter is primarily adapted from Sontag (1998) and Zhou (2017b).

4.1 The optimal control problem

In general, in an optimal control problem, we have a system of functions, written in *state space*,

$$\dot{x}(t) = f(x(t), u(t), t), x(0) = x_0.$$

where $t \to x : T \to \mathbb{R}^n$ and $t \to u : T \to \mathcal{U}$, where $\mathcal{U} \subseteq \mathbb{R}^m$ is a set of admissible controls (typically finite) and T is the set of time, which can be e.g. $T \subseteq \mathbb{R}$ (continuous time) or $T \subseteq \mathbb{N}$ (discrete time). We consider a *cost function* $J : T \times \mathbb{R}^n \times \mathcal{U} \to \mathbb{R}$ depending on the the instantaneous cost $q : T \times \mathbb{R}^n \times \mathcal{U} \to \mathbb{R}$,

$$J(t, x, u) = \int_{t_0}^{t_f} q(\eta, x(\eta), u(\eta)) d\eta + J_N(x(t_f)),$$

assigning to each possible sequence of controls and its corresponding states (this combination of a control and a state will sometimes be referred to as a trajectory), a cost. The term $J_N : \mathbb{R}^n \to \mathbb{R}$ is a cost that applies no matter what control is chosen. The cost function is equivalent to the functionals treated in Section 3. Naturally, we want to minimise the cost.

Optimal control theory can be broadly divided into two fields: dynamic programming, which deals with time-discrete problems, and variational methods, which are continuous in time. Since the problems considered here are naturally continuous in time (they can of course be discretised for numerical treatment, but there is no natural choice of such a time increment based on the problem itself) we will focus on the latter. However, for a comprehendible introduction it is impossible to leave out the time-discrete problems completely.

A peculiarity of optimal control is that problems are typically solved "backwards"; we know where we want to end up, so we work our way back from there, thereby performing the analysis backward in time.

4.2   Bellman's optimality principle and the Bellman equation

"An optimal policy has the property that whatever the initial state and initial decisions are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision." Bellman (1957)

Some problems are naturally discrete in time. For example, in the problem of an old-time traveller travelling with a horse-drawn coach between two distant cities pondering how to lay out her journey, it is implied that the traveller needs to stop and rest after one unit of time (one day). The Bellman equation, or dynamic programming, is a part of optimal control theory, which deals with problems that are discrete in time.

Suppose at a time $t \in T \subseteq \mathbb{N}$ we have a problem (say the traveller mentioned above) wanting to determine the control u_t (the choice of which town to travel to next). (In the case of the traveller, u_t is scalar, but as before, we can have $u_t \in \mathcal{U} \subseteq \mathbb{R}^m$.) The total accumulated cost (or total travel time) up to the time horizon is

$$J(t, x, u) = \sum_{t=0}^{N-1} J(x_t, u_t) + J_N(x_N).$$

And we can write the cost-to-go-function as

$$J_t(t, x, u) = \sum_{\tau=t}^{N-1} J(x_\tau, u_\tau, \tau) + J_N(x_N).$$

We want to optimise (minimise) the cost. To our help we have the principle of optimality which states that the optimal policy from $t = \tau$ to $t = N - 1$ is obtained by choosing the control that optimises J over each subinterval on $[\tau, N - 1)$. Assume that a sequence of controls $(u_{t+1}, u_{t+2}, ..., u_{N-1})$ are optimal for J_{t+1}. Then the optimal policy for J_t is to chose the control u_t that minimises J on the interval $[t, t + 1)$,

$$\inf_{u_t} J_t(t, x, u) = \inf_{u_t} \sum_{\tau=t}^{N-1} J(x_\tau, u_\tau) + J_N(x_N), \qquad (17)$$

which recursively leads to an optimal policy. When a minimum can be found using such a recursion the problem is said to have an optimal substructure. The equation (17) gives the optimal total cost if all stages after t are optimal. The recursion then goes back in time step by step. The strength of the optimality principle and the Bellman equation is that it breaks down the problem of finding an optimal

19

policy into a finite sequence of simpler problems. Now, consider the dynamical system,

$$x_{t+1} = f(x_t, u_t, t), \tag{18}$$

where $t \rightarrow x : T \rightarrow \mathbb{R}^n$ is the state variable, and $u_t \in \mathcal{U} \subseteq \mathbb{R}^m$ is the control, we assume that we know the sequence $U_t = (u_0, ..., u_{t-1})$ which determines the state of the system. Also assume that we have some cost function $J : T \times \mathbb{R}^n \times \mathcal{U} \rightarrow \mathbb{R}$

$$J(t, x, u) = \sum_{t=0}^{N-1} J(x_t, u_t, t) + J_N(x_N),$$

that should be minimised, by a proper choice of controls $u_0, ..., u_{N-1}$. And we write the minimal or optimal cost-to-go-function $V : T \times \mathbb{R}^n \rightarrow \mathbb{R}$ as

$$V(x_t) = \inf_{u_t, ..., u_{N-1}} J_t,$$

where x_t is $x(t)$. Here, $V(x, t)$ is a minimal future cost from time t and onwards. We can then construct the optimal cost-to-go function recursively using the principle of optimality, which gives us the Bellman equation.

Theorem 4.1 (The Bellman equation). *The optimal cost-to-go function at time t is given by*

$$V(x_t) = \inf_u [J(x, u, t) + V(f(x_t, u_t, t))], \quad t < N,$$

with terminal condition $V(x_N) = J_N(x_N)$.

Proof. The proof is by induction. At time $t = N - 1$, we have

$$V(x_{N-1}) = \inf_{u_{N-1}} J_{N-1}.$$

Taking one step backwards, at $t = N - 2$, we will have

$$V(x_{N-2}) = \inf_{u_{N-2}, u_{N-1}} J_{N-2} = \inf_{u_{N-2}} J_{N-2} + \inf_{u_{N-1}} V(x_{N-1}).$$

But by the state equation (18), $x_{N-1} = f(x_{N-2}, u_{N-2}, N-2)$ so

$$V(x_{N-2}) = \inf_{u_{N-2}} J_{N-2} + \inf_{u_{N-1}} V(f(x_{N-2}, u_{N-2}, N-2)).$$

At time t,

$$V(x_t) = \inf_{u_t} J_t + \inf_{u_{t-1}} V(f(x_t, u_t, t)).$$

So looking over the entire interval $t \in [0, N-1]$, we must have

$$V(x_t) = \inf_u [J(x, u, t) + V(f(x, u, t))].$$

$\square$

4.3 Hamilton-Jacobi-Bellman equations

In the previous subsection, we were only dealing with problems which are discrete in time. We will now derive the equivalent of the Bellman equation in continuous time, the Hamilton-Jacobi-Bellman equation. First, we define the optimality principle in continuous time.

Consider a dynamical system in continuous time,

$$\dot{x} = f(x, u, t), x(t_0) = x_0,$$

with a cost functional $J : T \times \mathbb{R}^n \times \mathcal{U} \to \mathbb{R}$, depending on the instantaneous cost $q : T \times \mathbb{R}^n \times \mathcal{U}$,

$$J(t_0, x_0, u) = \int_{t_0}^{t_f} q(x, u, t)dt + Q(x(t_f)),$$

where $t \to x : T \to \mathbb{R}^n$, $t \to u : T \to \mathcal{U} \subseteq \mathbb{R}^m$, and where $T \subseteq \mathbb{R}$ is the (continouous) set of time and $\mathcal{U}$ is a set of admissible controls. The term $Q : \mathbb{R}^n \to \mathbb{R}$ represents a cost that applies no matter what control is chosen. Then the cost-to-go-functional is

$$J_t(t, x, u) = \int_t^{t_f} q(x, u, \tau)d\tau + Q(x(t_f)).$$

and the optimal cost-to-go $V : T \times \mathbb{R}^n \to \mathbb{R}$ is

$$V(t, x) = \inf_u J_t(t, x, u).$$

The optimisation problem can thus be expressed: Find the controls $u(t)$ that give P as

$$P = \inf_u J(t_0, x_0, u).$$

Theorem 4.2 (The optimality principle in continuous time). *Let $u^* : [t_0, t_f] \to \mathcal{U} \subseteq \mathbb{R}^m$ be an optimal policy that minimises P, and that generates an optimal trajectory $x^* : [t_0, t_f] \to \mathbb{R}^n$. Then for any $t \in (t_0, t_f]$, the restriction of the optimal control to $[t, t_f]$, $u^*|_{[t,t_f]}$ is optimal for $\min_u J(t, x^*, u)$ and the corresponding optimal trajectory is $x^*|_{[t,t_f]}$.*

Proof. The proof is by contradiction. By additivity of integrals, the optimal cost is

$$V(t_0, x_0) = \int_{t_0}^t q(x^*, u^*, t)dt + J_t(t, x^*, u^*|_{[t,t_f]}).$$

Assume $u^*|_{[t,t_f]}$ is not optimal. Then there would exist admissible controls $\hat{u}$, defined only on $[t, t_f]$ such that

$$u(\tau) = \begin{cases} u^*(\tau) & \tau \in [t_0, t) \\ \hat{u}(\tau) & \tau \in [t, t_f], \end{cases}$$

and

$$J_t(t, x^*, \hat{u}) < J_t(t, x^*, u^*|_{[t,t_f]}).$$

21

The cost function related to this control is

$$J(t_0, x_0, \hat{u}) = \int_{t_0}^{t} q(x^*, u^*, t)dt + J_t(t, x^*, \hat{u})$$

$$< \int_{t_0}^{t} q(x^*, u^*, t)dt + J_t(t, x^*, u^*|_{[t,t_f]}) = V(t_0, x_0).$$

But $V(t_0, x_0)$ is the optimal cost to go, so we get a contradiction. Thus $u^*(\tau)|_{[t,t_f]}$ must be optimal for $\tau \in [t, t_f]$. $\qquad\square$

In order to formulate the Bellman equation in continuous time, we also need to redefine the minimal cost-to-go function in continuous time. If u^* is the optimal control function, then

$$V(x, t) = J(t, x, u^*).$$

In the time-discrete case, the optimal cost to go function would read

$$V(x, t) = \inf_u [q(x, u, t)\Delta + V(x + f(x, u, t)\Delta, t + \Delta)], \qquad (19)$$

with Δ being the time step of the discrete time problem in continuous time. By Taylor expansion of the last term of (19), we have

$$V(x + f(x, u, t)\Delta, t + \Delta) \approx V(x, t) + \frac{\partial V(x, t)}{\partial t}\Delta + \frac{\partial V(x, t)}{\partial x}f(x, u, t)\Delta,$$

provided that the partial derivatives of V exist. So

$$V(x, t) = \inf_u [q(x, u, t)\Delta + V(x, t) + \frac{\partial V(x, t)}{\partial t}\Delta + \frac{\partial V(x, t)}{\partial x}f(x, u, t)\Delta].$$

Now, $V(x, t)$ is independent of u, and can be moved outside the minimisation. Subtracting $V(x, t)$ in both sides gives the Hamilton-Jacobi-Bellman equation, also known as dynamic programming in continuous time,

$$\frac{\partial V(x, t)}{\partial t} + \inf_{u \in U} \left[q(x, u, t) + \frac{\partial V(x, t)}{\partial x}f(x, u, t) \right] = 0. \qquad (20)$$

4.4   Pontryagin's minimum principle

Pontryagin's minimum principle is a necessary condition for an optimal trajectory. The main benefit of Pontryagin's minimum principle is that its equations are simpler to work with than the Hamilton-Jacobi-Bellman equations. Assume that we have a dynamical – although time-invariant – system with $t \to x : T \to \mathbb{R}^n$, $t \to u : T \to \mathcal{U} \subseteq \mathbb{R}^m$,

$$\dot{x} = f(x, u), x(t_0) = x_0,$$

along with a cost functional $J : T \times \mathcal{U} \times \mathbb{R}^n \rightarrow \mathbb{R}$, depending on the instantaneous cost $q : T \times \mathcal{U} \times \mathbb{R}^n \rightarrow \mathbb{R}$ and the residual cost $Q : \mathbb{R}^n \rightarrow \mathbb{R}$ of the form

$$J(t_0, x_0, u) = \int_{t_0}^{t_f} q(x, u, t)dt + Q(x(t_f)),$$

Disregard for a minute the dependence of J on t and x. Assuming that $J(u)$ satisfies the property that if both u and $u + \delta u$ are two admissible controls, and assuming that δ is small, then

$$\Delta J = J(u + \delta u) - J(u) = \delta J(u, \delta u) + j(u, \delta u)||\delta u||.$$

This is equivalent to saying that J has a (partial) Gâteaux derivative with respect to u. Note that δJ is linear in δu and that $j(u, \delta u) \rightarrow 0$ as $\delta u \rightarrow 0$. If $u = u^*$ is an extremal, then there exists an $\epsilon > 0$ such that for all $||u - u^*|| < \epsilon$, $J(u) - J(u^*) \geq 0$. Then the following theorem, which is equivalent to Theorem 3.1 (and therefore left without proof) will show to be very useful

Theorem 4.3. *(Zhou (2017b)) A necessary condition for u^* to be an extremal is that $\delta J(u^*, \delta u) = 0$ for all δu.*

Now as a trick, we introduce a vector (possibly of length 1) of Lagrange multipliers $x \rightarrow p : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $p = (p_1, ..., p_n)^T$ and form the augmented functional

$$J = Q(x(t_f)) + \int_{t_0}^{t_f} \left(q(x, u, t) + p^T(f - \dot{x}) \right) dt.$$

Since $\dot{x} = f$, this does not alter the equality. Integrating the last term by parts gives

$$J = Q(x(t_f)) - [p^T x]_{t_0}^{t_f} + \int_{t_0}^{t_f} \left(H + \dot{p}^T x \right) dt,$$

where $H : \mathbb{R}^n \times \mathcal{U} \times T \times \mathbb{R}^n \rightarrow \mathbb{R}$, $H(x, u, t, p) = q(x, u, t) + p^T f$ is called the Hamiltonian function. Assume that $f, q, p \in C^1$ on x and continuous in u. Then the first variation $\delta J = 0$ is a necessary condition for u^* to be an extremal, which is what is stated in Pontryagin's minimum principle.

Theorem 4.4 (Pontryagin's minimum principle)**.** *A necessary condition for u^* to be an extremal for the optimal control problem is that*

$$\delta J = \left[\left(\frac{\partial Q}{\partial x} - p^T \right) \delta x \right]_{t=t_f} + \int_{t_0}^{t_f} \left[\frac{\partial H}{\partial x} \delta x + \frac{\partial H}{\partial u} \delta u + \dot{p}^T \delta x \right] dt = 0,$$
(21)

where δx is a variation in x in the differential equation due to the variation in u.

Proof. The proof follows directly from Theorem 4.3. □

Remark 4.1. *Pontryagin's minimum principle is often written in more condensed form as*

(i) $\dot{p}_i = -\frac{\partial H}{\partial x}, i = 1, 2, ..., n,$

(ii) $p_i(t_f) = \left(\frac{\partial Q}{\partial x_i} \right)_{t=t_f},$

(iii) $\left(\frac{\partial H}{\partial u_i} \right)_{u=u^*} = 0.$

This follows from (21) above. Equating the terms involving δx leads to (i) and (ii). above. Then (21) reduces to $\delta J_a = \int_{t_0}^{t_f} \left(\frac{\partial H}{\partial u_i} \delta u \right) dt$ and since δu is an arbitrary variation, (iii) follows from the fundamental lemma of calculus of variations.

4.5 Application to the gradient regularised damage models in uniaxial tension

In physics, behaviour with respect to time often differs significantly from behaviour with respect to space, and interchanging these would be at best amusing. Mathematics, on the other hand, does not discriminate with respect to the choice of variables. We can therefore formulate the control problems with respect to x, rather than time. We also know that there is no energy stored outside of the elastic body, thus $J_N = 0$.

4.5.1 Gradient regularised damage model with an elastic phase

We turn again to the uniaxial tension of the bar using the gradient regularised damage model with $w = w_1 d$ and $E = E_0(1-d)^2$. Consider the bar $\Omega = S \times [0, L]$, subjected to end displacement $U(0) = 0$ and $U(L) = tL$ (Fig. 1). Let $v = d'$ and let $[t, v]^T$ be our control. From the problem formulation (Section 1.1) we get the state equation

$$\begin{cases} u' = t, \\ d' = v. \end{cases}$$

We had the cost functional (10)

$$W(u, d) = S \int_0^L \left(w_1 d + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0 (1-d)^2 \left(u' \right)^2 \right) dx.$$

Introducing the multiplier, $[p_u, p_d]^T$ and using t and v instead of u' and d', the hamiltonian is

$$H(u, d, t) = w_1 d + \frac{1}{2} w_1 l^2 v^2 + \frac{1}{2} E_0 (1-d)^2 t^2 + p_u t + p_d v.$$

By Pontryagin's minimum principle (Theorem 4.4)

$$-p_u' = \frac{\partial H}{\partial u} = 0, \quad p_u(L) = 0, \tag{22}$$

$$-p_d' = \frac{\partial H}{\partial d} = w_1 - E_0(1-d)t^2, \quad p_d(L) = 0, \tag{23}$$

$$\frac{\partial H}{\partial t} = E_0(1-d)^2 t + p_u, \text{ and} \tag{24}$$

$$\frac{\partial H}{\partial v} = w_1 l^2 v + p_d. \tag{25}$$

If we differentiate (29) and insert into (27), we get the Euler-Lagrange equation (12) from the previous section. Also since (26) menas that $p_u = 0$, so $d/dx\left(E_0(1-d)^2 u'\right) = 0$ which is the Euler-Lagrange equation with respect to u (11). So we see that we get the same expressions for t_c, U_c, d etc. as we did in Subsection 3.3.3, that is, we find the same extremal using Pontryagin's minimum principle as we did using the Euler-Lagrange equation.

4.5.2 Gradient regularised damage model without elastic phase

Now, we consider the gradient regularised damage model with $w = w_1 d^2$ and $E = E_0(1-d)^2$ with the same state and control as in the previous section. We had the cost functional (10)

$$W(u,d) = S \int_0^L \left(w_1 d^2 + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0(1-d)^2 \left(u'\right)^2\right) dx.$$

Introducing the multiplier, $[p_u, p_d]^T$, the hamiltonian is

$$H(u,d,t) = w_1 d^2 + \frac{1}{2} w_1 l^2 v^2 + \frac{1}{2} E_0(1-d)^2 t^2 + p_u t + p_d v.$$

By Pontryagin's minimum principle (Theorem 4.4)

$$-p_u' = \frac{\partial H}{\partial u} = 0, \quad p_u(L) = 0, \tag{26}$$

$$-p_d' = \frac{\partial H}{\partial d} = 2w_1 d - E_0(1-d)t^2, \quad p_d(L) = 0, \tag{27}$$

$$\frac{\partial H}{\partial t} = E_0(1-d)^2 t + p_u, \text{ and} \tag{28}$$

$$\frac{\partial H}{\partial v} = w_1 l^2 v + p_d. \tag{29}$$

Again, we see that we get the Euler-Lagrange equation (15). Hence, we also get the same expressions for t_M, U_M, d etc. as we did in Section 3.3.4.

5 The second variation

Both the Euler-Lagrange equation (Theorem 3.2) and Pontryagin's minimum principle (Theorem 4.4) give only necessary conditions for J to be a minimum. In order to verify whether the extremals (stationary points which are not minima/maxima of J are still called extremals, van Brunt (2006)) are in fact minima, we need some additional theory, which is developed in this section. The theoretical material in this section is adapted from van Brunt (2006) and the application to the uniaxial tension problem is adapted from Benallal and Marigo (2007) and Pham et al. (2011).

5.1 Sufficient condition for the existence of minimisers

To continue the analogy with calculus: if we want to find a local minimum of a function, a necessary condition is that the derivative is zero. However, a sufficient condition is that the function value in a specific point is smaller than all other function values in a neighbourhood, i.e. for a function $x \to f : \mathbb{R} \to \mathbb{R}$

$$f(x_0) < f(x_0 + \epsilon),$$

where $\epsilon \in \mathbb{R}$ is small.

In order to verify that x is indeed a local minimum, we use Taylor expansion around the point x_0,

$$f(x_0 + \epsilon) = f(x_0) + \epsilon f'(x_0) + \frac{\epsilon^2}{2} f''(x_0) + O(\epsilon^3).$$

We know from the necessary conditions that $f'(x_0) = 0$, so

$$f(x_0 + \epsilon) - f(x_0) = \frac{\epsilon^2}{2} f''(x_0) + O(\epsilon^3),$$

that is, if the second-order derivative of f is positive, then f has a minimum at x_0. We will now prove the equivalent for functionals. Consider the functional $J : A \to \mathbb{R}, J(y) = \int_{x_0}^{x_1} f(x, y, y') dx$, where $A \subseteq V$, where V is a normed vector space of functions and $f : \mathbb{R} \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. Further suppose that $\epsilon v \in A$, and suppose that ϵ is small. We define the second variation of J as

$$\delta^2 J(y_0, v) = \int_{x_0}^{x_1} \left(v^2 \frac{\partial^2 f}{\partial y_0^2} + 2vv' \frac{\partial^2 f}{\partial y_0 \partial y_0'} + v'^2 \frac{\partial^2 f}{\partial y_0'^2} \right) dx. \qquad (30)$$

Theorem 5.1. *Suppose that the functional $J : A \to \mathbb{R}$ where $A \subseteq V$, where V is a normed vector space of functions. Further suppose that for a certain $y_0 \in A$, $\delta J(y_0) = 0$, i.e. that J has an extremal for y_0. If y_0 is a local minimiser of J, then*

$$\delta^2 J(y_0, \epsilon v) > 0,$$

for all small $\epsilon \in \mathbb{R}$.

Proof. Assume $J(y) = \int_{x_0}^{x_1} f(x, y, y')dx$ has an extremum for y_0 and consider a "nearby" function $\hat{y} = y_0 + \epsilon v$. The Taylor expansion of the function f is

$$f(x, \hat{y}, \hat{y}') = f(x, y_0, y_0') + \epsilon \left(v\frac{\partial f}{\partial y_0} + v'\frac{\partial f}{\partial y_0'} \right)$$
$$+ \frac{\epsilon^2}{2} \left(v^2\frac{\partial^2 f}{\partial y_0^2} + 2vv'\frac{\partial^2 f}{\partial y_0 \partial y_0'} + v'^2\frac{\partial^2 f}{\partial y_0'^2} \right) + O(\epsilon^3).$$

Using the second variation (Eq. (30)), we see that the difference between $J(y_0)$ and $J(\hat{y})$ can be rewritten as

$$J(y_0 + \epsilon v) - J(y_0) = \epsilon \delta J(y_0, v) + \frac{\epsilon^2}{2}\delta^2 J(y_0, v) + O(\epsilon^3).$$

Since the first variation is zero, the sign of the difference depends on the sign of the second variation, which is what is stated in the theorem. $\square$

We also want to derive this condition for functionals of two functions. Consider the functional $J : A \times A \to \mathbb{R}$ with $J(u, v) = \int_{x_0}^{x_1} f(x, u, u', v, v')dx$ where $f : \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. Again, $A \subseteq V$, where V is a normed vector space of functions. We define the second variation of $J(u, v)$,

$$\delta^2 J(u_0, v_0)(\epsilon h, \epsilon k) = \int_{x_0}^{x_1} \left(h^2\frac{\partial^2 f}{\partial u_0^2} + 2hh'\frac{\partial^2 f}{\partial u_0 \partial u_0'} + h'^2\frac{\partial^2 f}{\partial u_0'^2} \right.$$
$$+ 2hk\frac{\partial^2 f}{\partial u_0 \partial v_0} + 2hk'\frac{\partial^2 f}{\partial u_0 \partial v_0'} + 2h'k\frac{\partial^2 f}{\partial u_0' \partial v_0} + 2h'k'\frac{\partial^2 f}{\partial u_0' \partial v_0'} + k^2\frac{\partial^2 f}{\partial v_0^2}$$
$$\left. + 2kk'\frac{\partial^2 f}{\partial v_0 \partial v_0'} + k'^2\frac{\partial^2 f}{\partial v_0'^2} \right)dx,$$

where $\epsilon h \in A, \epsilon k \in A$ and ϵ is small.

Theorem 5.2. *Suppose that $J : A \times A \to \mathbb{R}$ depends on not one but two functions, $J(u, v)$, and suppose that $\delta J(u_0, v_0) = 0$, i.e. that J has a local extremum for u_0, v_0. If this extremum is a local minimum, then*

$$\delta^2 J(u_0, v_0)(\epsilon h, \epsilon k) > 0$$

for all $\epsilon h \in A, \epsilon k \in A$ and ϵ small.

Proof. Let $J(u, v) = \int_{x_0}^{x_1} f(x, u, u', v, v')dx$. We know that J is stationary for (u_0, v_0), so consider a nearby state $(\hat{u}, \hat{v}) = (u_0 + \epsilon h, v_0 + \epsilon k)$. The Taylor expansion of f is

$$f(x, \hat{u}, \hat{u}', \hat{v}, \hat{v}') = f(x, u_0, u_0', v_0, v_0')$$

$$+\epsilon \left(h \frac{\partial f}{\partial u_0} + h' \frac{\partial f}{\partial u_0'} + k \frac{\partial f}{\partial v_0} + k' \frac{\partial f}{\partial v_0'} \right)$$

$$+\frac{\epsilon^2}{2} \left(h^2 \frac{\partial^2 f}{\partial u_0^2} + 2hh' \frac{\partial^2 f}{\partial u_0 \partial u_0'} + h'^2 \frac{\partial^2 f}{\partial u_0'^2} + 2hk \frac{\partial^2 f}{\partial u_0 \partial v_0} + 2hk' \frac{\partial^2 f}{\partial u_0 \partial v_0'} \right.$$

$$\left. + 2h'k \frac{\partial^2 f}{\partial u_0' \partial v_0} + 2h'k' \frac{\partial^2 f}{\partial u_0' \partial v_0'} + k^2 \frac{\partial^2 f}{\partial v_0^2} + 2kk' \frac{\partial^2 f}{\partial v_0 \partial v_0'} + k'^2 \frac{\partial^2 f}{\partial v_0'^2} \right)$$

$$+O(\epsilon^3).$$

The proof follows from the previous one, as $\delta J(u, v) = 0$ implies that the first variation with respect to both functions u and v be zero. Then the first-order terms must be zero, and the difference between the functional value in $\hat{u}, \hat{v}$ and u_0, v_0 is given by the second variation. $\square$

5.2 Application to the gradient regularised damage models in uniaxial tension

We now turn to the application of the tension of a rod. We recall that the first variation of the first model was not zero in the elastic region, whereas the Euler-Lagrange equation was always fulfilled for the second model, which did not have an elastic phase.

5.2.1 Gradient regularised damage model with an elastic phase

We recall Eq. (10),

$$W(u, d) = S \int_0^L \left(w_1 d + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0 (1 - d)^2 (u')^2 \right) dx.$$

First, remember that in the elastic phase $(tx, 0)$ the first variation of $W(u, d)$ was not zero. But the first variation around the homogenous state $d(x) = 0$ and $u(x) = u_t = tx$ in direction β and v,

$$\delta J(tx, 0), (v, \beta) = S \int_0^L (v' E_0^2 u' + \beta(w_1 + E_0 u'^2)) dx.$$

is positive by virtue of $w_1 > 0$, $E_0 > 0$, $u' > 0$, $\beta \in [0, 1]$ and the fact that we must have $v' E_0^2 u' = 0$ (since this is the first variation of the purely elastic problem, cf. Section 3.3.3). Hence the elastic phase must be stable, since this first variation term is larger than the second variation term in the Taylor expansion.

In the damaging phase, the first variation is zero. The second variation of Eq. (10) around the homogenous state $d(x) = d_t$ and $u(x) = u_t = tx$ in direction β and v is

$$\delta^2 J\left(u_t, d_t\right), (v, \beta) = S \int_0^L \left(v'^2 E_0(1-d)^2 - 4v'\beta E_0(1-d)u'\right. \tag{31}$$
$$\left. + \beta^2 E_0 u'^2 + \beta'^2 w_1 l^2\right) dx.$$

If this quantity is strictly greater than zero, then the homogenous solution is stable. We can rewrite (31) (using the relation $u' = t$)

$$\delta^2 J\left(u_t, d_t\right), (v, \beta) = S \int_0^L \left(\beta'^2 w_1 l^2 + E_0(1-d)^2 \left(v' - \frac{2t\beta}{(1-d)}\right)^2\right.$$
$$\left. - 3 E_0 t^2 \beta^2\right) dx.$$

To verify whether the second variation is positive, it is necessary to know which terms are positive. Since E_0 and w_1 are positive, the first and second terms are positive due to the squares. If the last term also is positive the homogenous state is a minimum, but the last term is negative. Then a condition for a minimum is that the absolute values of the last term is smaller than the other terms, i.e. that the functional

$$\mathcal{R} = \frac{\int_0^L \left(w_1 l^2 \beta'^2 + E_0(1-d)^2 \left(v' - \frac{2t}{(1-d)}\beta\right)^2\right) dx}{\int_0^L 3 E_0 t^2 \beta^2 dx} > 1.$$

By proposition A2 by Pham et al. (2011) (the proof is outside the scope of this thesis), the minimum of a functional of the form

$$\mathcal{R} = \frac{\int_0^1 a\beta'^2 + b(v' - c\beta)^2 dx}{\int_0^1 \beta^2 dx}$$

is governed by the minimum of bc^2 and $\pi^2 a$ such that

$$\begin{cases} \text{if } \pi^2 a > bc^2 \text{ then } \min \mathcal{R} = bc^2, \\ \text{if } \pi^2 a = bc^2 \text{ then } \min \mathcal{R} = bc^2, \\ \text{if } \pi^2 a < bc^2 \text{ then } \min \mathcal{R} = (\pi^2 a)^{1/3}(bc^2)^{2/3}. \end{cases} \tag{32}$$

Observing that $a = l^2 w_1/(3E_0 t^2)$, $b = (1-d)^2/(3t^2)$, and $c = 2t/(1-d)$, and changing the variable from x to x/L, after some rather long but standard calculations, we find that $\mathcal{R}$ has minimum

$$\begin{cases} \frac{4}{3}, & \text{if } \frac{\pi^2 w_1}{3E_0 t^2} \frac{l^2}{L^2} \geq \frac{4}{3}, \\ \left(\frac{\pi^2 w_1}{3E_0 t^2}\right)^{1/3} \left(\frac{4}{3}\right)^{2/3} \left(\frac{l}{L}\right)^{2/3}, & \text{otherwise.} \end{cases}$$

The first case is always stable, since $4/3 > 1$. The second case is stable if and only if the length of the bar is sufficiently small. We know that $\sqrt{w_1/E_0} = t_c$. Finally we arrive at a critical length L_s, i.e. the damage evolution is stable if and only if $L < L_s$ with

$$L_s = \frac{4l\pi}{3\sqrt{3}} \frac{t_c}{t}.$$

In terms of fracture mechanics, this means that the damage will localise into a crack and the rod will break. If $L < L_s$ and the damage evolution is stable, then by Eq. (13) and Fig. 4, the rod will weaken but continue to carry load for all finite displacements.

Remark 5.1. *The Hamilton-Jacobi-Bellman equation (Eq. 20) gives both necessary and sufficient conditions for optimality. The Hamilton-Jacobi-Bellman equation may be difficult or even impossible to solve, but we can check that it is fulfilled. Note that the cost-to-go function $V(u, d, x)$ can be written*

$$V(u, d, x) = \min_{t,v} \int_x^L w_1 d + \frac{1}{2} E_0 (1-d)^2 t^2 + \frac{1}{2} w_1 l^2 v^2 dx.$$

If we insert $d = (1 - w_1/(E_0 t^2))$ and $d' = v = 0$ and evaluate we get

$$V(u, d, x) = w_1 d(L - x) + \frac{1}{2} E_0 (1-d)^2 t^2 (L - x) \ \ or$$

$$V(u, d, x) = w_1 (L - x) - \frac{w_1^2}{2E_0 t^2}(L - x).$$

We then get the Hamilton-Jacobi-Bellman equation as

$$\min_{t,v} \left(w_1 \left(1 - \frac{w_1}{E_0 t^2} \right) + \frac{w_1^2}{2E_0 t^2} + (w_1 (L - x) - w_1) d' \right)$$

$$= w_1 - \frac{1}{2} \frac{w_1^2}{E_0 t^2} = -\frac{\partial V}{\partial x}.$$

so the Hamilton-Jacobi-Bellman equation is fulfilled for the previously obtained solution as long as the assumption $d'' = 0$ is valid. This does not contradict the condition above. For short bars the damage will not localise and the assumption is valid. For longer bars, damage will localise and the damage is no longer constant.

5.2.2 Gradient regularised damage model without elastic phase

We recall Eq. (14),

$$W(u, d) = S \int_0^L \left(w_1 d^2 + \frac{1}{2} w_1 l^2 d'^2 + \frac{1}{2} E_0 (1-d)^2 (u')^2 \right) dx.$$

For this model there is no need to separate the analysis into different phases, as there is only one phase. The first variation is always zero.

The second variation around the homogenous state $d(x) = d_t$ and $u(x) = u_t = tx$ in direction β and v is

$$\delta^2 J\left(u_t, d_t\right), (v, \beta) = S \int_0^L \left(v'^2 E_0 (1-d)^2 - 4v'\beta E_0 (1-d)u' \right.$$
$$\left. + \beta^2 (2w_1 + E_0 u'^2) + \beta'^2 w_1 l^2 \right) dx.$$

Again, we can rewrite (using $u' = t$),

$$\delta^2 J\left(u_t, d_t\right), (v, \beta) = S \int_0^L \left(\beta'^2 w_1 l^2 + E_0 (1-d)^2 \left(v' - \frac{2t\beta}{(1-d)}\right)^2 \right.$$
$$\left. - (3E_0 t^2 - 2w_1)\beta^2 \right) dx.$$

By the same argument as before, the condition for stability is that

$$\mathcal{R} = \frac{\int_0^L \left(w_1 l^2 \beta'^2 + E_0 (1-d)^2 \left(v' - \frac{2t}{(1-d)}\beta\right)^2\right) dx}{\int_0^L (3E_0 t^2 - 2w_1)\beta^2 dx} > 1.$$

Observing that $a = w_1 l^2 / (3E_0 t^2 - 2w_1)$, $b = E_0 (1-d)^2 / (3E_0 t^2 - 2w_1)$ and $c = 2t/(1-d)$, we can use (32) to obtain the minimum of $\mathcal{R}$ as:

$$\begin{cases} \frac{4E_0 t^2}{3E_0 t^2 - 2w_1}, & \text{if } \pi^2 w_1 \left(\frac{l}{L}\right)^2 \geq 4E_0 t^2, \\ \frac{(\pi^2 w_1)^{1/3}(4E_0 t^2)^{2/3}}{3E_0 t^2 - 2w_1} \left(\frac{l}{L}\right)^{2/3}, & \text{otherwise.} \end{cases}$$

The first case is always stable, since we have $w_1 \in [0, \infty)$. If $2w_1 > 3E_0 t^2$ all terms in the second variation would be positive, and if $2w_1 < 3E_0 t^2$ we have the quotient larger than 1. The second case, using the relation $t_M = \sqrt{(2w_1)/(3E_0)}$, gives the condition that damage evolution is stable if and only if

$$L < L_s = \frac{l\pi 2\sqrt{2}}{3} \frac{t^2/t_M^2}{(t^2/t_M^2 - 1)^{3/2}}.$$

Again, the stability criterion is not universally fulfilled but rather depends on the length of the rod. In the region $t < t_M$, the solution is stable. In the stress-softening region after $t = t_M$, the solution is only stable if the length of the rod is smaller than L_s, but for $L > L_s$ damage will localise and form a crack.

Remark 5.2. *Using the Hamilton-Jacobi-Bellman equation (Eq. 20), we write the cost-to-go function $V(u, d, x)$ as*

$$V(u, d, x) = \min_{t,v} \int_x^L w_1 d^2 + \frac{1}{2} E_0 (1-d)^2 t^2 + \frac{1}{2} w_1 l^2 v^2 dx.$$

If we use $d' = v = 0$ and evaluate we get

31

$$V(u, d, x) = w_1 d^2 (L - x) + \frac{1}{2} E_0 (1 - d)^2 t^2 (L - x).$$

We then get the Hamilton-Jacobi-Bellman equation as

$$\min_{t,v} \left(w_1 d^2 + \frac{1}{2} E_0 (1 - d)^2 t^2 \right) = -\frac{\partial V}{\partial x}.$$

so the Hamilton-Jacobi-Bellman equation is fulfilled for the previously obtained solutions as long as the assumption $d'' = 0$ is valid.

6 Conclusions

We have investigated three different models for fracture of materials mathematically. The older of the models, Griffith's model predicts that fracture will never occur, unless there is already a crack in a body. The younger models, the variational approach and the gradient regularised models, predict fracture also in initially undamaged bodies.

In general, it is not possible to obtain solutions to the variational approach problem; in fact, only a few problems have known solutions. (In addition to the one-dimensional tension problem studied here, these are the equivalent of the one-dimensional tension but with deformation of the rod described in three dimensions, and separation of a cylindrical reinforcement.)

The gradient regularised models allow for easier analytical and – primarily – numerical treatment. The gradient regularised models introduce a new variable, as well as an additional constant with dimension length. Thanks to this reformulation, approximate (numerical) solutions can be obtained for a very wide range of problems, using e.g. the traditional methods from calculus of variations (i.e. the Euler-Lagrange equation). Here, we circumvent the issue of having to use numerical analysis to solve the resulting partial differential equation by making certain assumptions on the second derivative of the damage variable, assumptions that are however only valid in the specific toy problem studied.

When using optimal control theory and specifically Pontryagin's minimum principle, we obtain the same solutions as we did using the Euler-Lagrange equation. The main benefit of Pontryagin's minimum principle is that it is in some senses more general than the Euler-Lagrange equation. It does not pose the same requirements on C^2 continuity of the Lagrangian, instead it poses requirements on C^1 continuity on several of the functions involved. Pontryagin's minimum principle is also able to handle constraints on the state or control variables (not shown in this essay).

The Euler-Lagrange equation and Pontryagin's principle give only necessary conditions for a the existence of minimisers. We have also derived sufficient conditions using the second variation. Application to the one-dimensional tensile test shows that solutions to the problem of gradient regularised damage in one-dimensional tension are indeed minimisers and thus observable and stable in an initial stress-hardening phase, but possibly unstable in the subsequent stress-softening phase. For short bars, the solution is always a minimiser.

The Hamilton-Jacobi-Bellman equation is a necessary and sufficient condition for optimality but the partial differential equation is difficult to solve. When we use it to verify the solutions obtained with the other methods, we find that as long as the assumption on the second derivative of the damage variable holds, the solutions are indeed minimisers. The physical interpretation of the sufficient conditions for optimality is that for short bars the damage will not localise and the assumption on the second derivative of the damage variable is valid. For longer bars,

damage will localise, meaning that the damage is no longer constant over the length of the bar and the obtained solutions are no longer minimisers.

Bibliography

Bellman, R. (1957). *Dynamic Programming.* Princeton University Press, New Jersey.

Benallal, A. and Marigo, J. J. (2007). Bifurcation and stability issues in gradient theories with softening. *Modelling and simulation in materials science and engineering*, 15:283–295.

Francfort, G. and Marigo, J. J. (1998). Revisiting brittle fracture as an energy minimization problem. *Journal of the Mechanics and Physics of Solids*, 46(8):1319–1342.

Francfort, G. and Marigo, J. J. (1999). Cracks in fracture mechanics : A time indexed family of energy minimizers. In Argoul, P., Frémond, M., and Nguyen, Q. S., editors, *IUTAM Symposium on Variations of Domain and Free-Boundary Problems in Solid Mechanics*, pages 197–202, Dordrecht. Springer, Netherlands.

Griffith, A. A. (1921). The Phenomena of Rupture and Flow in Solids. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 221(582–593):163–198.

Hilbert, D. (1902). Mathematical problems. *Bulletin of the American Mathematical Society*, 8:437–479.

Logan, D. (2013). *Applied Mathematics.* John Wiley and Sons, New York.

Marigo, J. J., Maurini, C., and Pham, K. (2016). An overview of the modelling of fracture by gradient damage models. *Meccanica*, 51(12):3107–3128.

Pham, K., Amor, H., Marigo, J. J., and Maurini, C. (2011). Gradient Damage Models and Their Use to Approximate Brittle Fracture. *International Journal of Damage Mechanics*, 20(4):618–652.

Sontag, E. D. (1998). *Mathematical Control Theory: Deterministic Finite Dimensional Systems.* Springer, New York.

van Brunt, B. (2006). *The calculus of variations.* Springer, New York.

Zhou, Y. (2017a). The brachistochrone problem. Lecture notes.

Zhou, Y. (2017b). Optimal control theory in mathematical modelling. Lecture notes.