Something Mathy

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Abstract

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Introduction

Chapter 1

Background

1.1 PDE Discretization

Multidimensional topological optimization problems often involve the use of partial differential equations (PDEs) which model the physical properties of the materials involved. Most of these PDEs cannot be uniquely solved analytically, so we turn to numerical methods in order to approximate their solutions. The first step in many of these methods is to discretize our domain; that is, we want to choose some scheme to divide our continuous domain into a finite number of pieces over which we will apply a particular method to approximate solutions to the PDE.

In the SIMP method, the Finite Volume Method is used to discretize and approximate solutions to the heat equation for our heat generating medium. We will introduce the Heat Equation and then proceed to give an overview of the Finite Volume Method.

1.1.1 The Heat Equation

Consider a stationary object of that has heat flowing between its interior regions. The temperature at any point in the interior of the object will depend on the spatial position chosen as well as the time we measure the temperature at that point. Therefore, the temperature (T) at any point in such an object is a function of both space (\vec{x}) and time (t) coordinates: $T(\vec{x},t)$. Physical principles demand that such a temperature function must satisfy the equation

$$\frac{\partial T}{\partial t} = \nabla \cdot \left(k(\vec{x}) \nabla T \right),\tag{1.1}$$

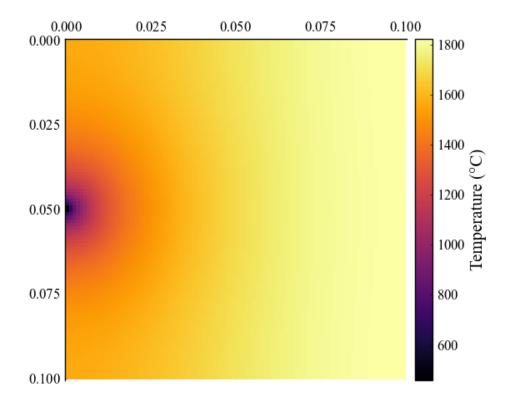


Figure 1.1: Heatmap for a $0.1 \text{ m} \times 0.1 \text{ m}$ object with uniform heat generation and a heat sink at the center of its west boundary. This map was produced via the Finite Volume Method using 100×100 uniform control volumes.

where ∇ is the gradient operator and the function k represents the thermal diffusivity at a point in our object.

Equation (1.1) is commonly referred to as the Heat or Diffusion Equation. If we were to have a constant thermal diffusivity throughout our object, it would be possible to analytically find a solution to this partial differential equation. However, as in the problems of interest throughout this paper, when k is not constant we must turn to numerical methods to find approximate solutions for the function T.

1.1.2 The Finite Volume Method

For our numerical approximations of PDEs in this paper we used the Finite Volume Method (FVM), which will be described in this section.

As with any other numerical method to solve PDEs, we must first discretize our domain by creating some sort of mesh. One major advantage of the Finite Volume Method is that we have a great amount of freedom in choosing our mesh. In FVM the domain can be discretized into a mesh of arbitrary polygons, but we chose uniform squares in our work to simplify the resulting calculations.

Given a mesh of polygons on our domain Ω with vertices at $\{x_i\} \subset \Omega$, we create a set of *control volumes* around each x_i . The resulting set of control volumes discretize the partial differential equation. The Finite Volume Method has us integrate our PDE over each control volume and then use the Divergence Theorem to convert these volume integrals into surface integrals involving the fluxes across the boundaries of the control volumes. We then approximate those fluxes across the boundaries to calculate approximate solutions to our PDE.

Theorem 1 (The Divergence Theorem). Suppose that V is a compact subset of \mathbb{R}^n that has a piecewise smooth and positively oriented boundary S (i.e. $\partial V = S$). If \mathbf{F} is a continously differentiable vector field defined on a neighborhood of V, then

$$\iiint_{\mathcal{V}} (\nabla \cdot \mathbf{F}) \, d\mathcal{V} = \oiint_{\mathcal{S}} \mathbf{F} \cdot d\mathcal{S}. \tag{1.2}$$

The divergence theorem is the key component in the finite volume method because it allows us to look at fluxes across the boundaries of each control volume, rather than the control volume itself.

Let's look at the finite volume method applied to the heat equation in two dimensions. Suppose we have discretized our space by dividing it up into a mesh of control volumes $\{V_i\}$. We integrate the heat equation PDE over each control volume, using the divergence theorem to convert the volume integral into a surface integral:

$$\int_{V_i} \frac{\partial T}{\partial t} d\vec{x} = \int_{V_i} \nabla \cdot \left(k(\vec{x}) \nabla T \right) d\vec{x} = \int_{\partial V_i} k(\vec{x}) \nabla T \cdot ds,$$

where *s* represents the lines that form the boundary of the control volume. Then, applying an approximation scheme to this result, we obtain a sparse and structured linear system.

One other major advantage of the finite volume method is that boundary conditions can easily be taken into account on general domains. For example, adding a heat sink by applying a Dirichlet boundary condition ($T_s = 0$ °C) can be thought of as zeroing out our algebraic equations by introducing a ghost cell that, when interpolated with the boundary cell, causes the temperature across the boundary to be zero.

1.2 The Optimization Problem

In much of mathematics, our goal is to seek some sort of solution. In cases where there are multiple solutions, it is desirable to determine the "best" solution judged against some set of criteria. Mathematical optimization is the study of solving such problems. In its simplest case, mathematical optimization is the practice of minimizing or maximizing a given function over a certain set and possibly subject to some constraints.

Definition 1. An optimization problem (in standard form) has the form

minimize
$$f_0(x)$$

subject to $f_i(x) \le 0$, $i = 1, ..., m$ (1.3)
 $h_i(x) = 0$, $i = 1, ..., p$

where

- $x = (x_1, ..., x_n)$ are the optimization variables,
- $f_0: \mathbb{R}^n \to \mathbb{R}$ is the objective function,
- $f_i: \mathbb{R}^n \to \mathbb{R}$ are the inequality constraint functions, and

• $h_i: \mathbb{R}^n \to \mathbb{R}$ are the equality constraint functions.

If there are no constraints (m = p = 0), then the problem is called *unconstrained*. (Boyd & Vandenberghe, 2004, p. 127)

We call a vector x^* **optimal** if it has the smallest objective value among all vectors that satisfy the constraints. That is, for any z with $f_1(z) \le 0, \ldots, f_m(z) \le 0$, then $f_0(z) \ge f_0(x^*)$. A point x that is in the domains of each function f_i and h_i is called **feasible** if it satisfies all the constraints. Finally, the **optimal value** p^* of the problem is defined as

$$p^* = \{f_0(x) \mid f_i(x) \le 0, i = 1, \dots, m, h_i(x) = 0, i = 1, \dots, p\}.$$

Therefore, $p^* = f_0(x^*)$, the objective function value at a feasible, optimal vector x^* .

Notice that the optimization problem in standard form is a minimization problem. We can easily change it into a maximization problem by minimizing the objective function $-f_0$ subject to the same constraints.

The optimization problem is **linear** or called a **linear program** if the objective and constraint functions are all linear. An optimization problem involving a quadratic objective function and linear constraints is **quadratic** or a **quadratic program**. If the optimization problem is not linear or quadratic, it is referred to as a **nonlinear program**.

There are exists efficient methods for solving linear programming and many quadratic programming problems.

1.2.1 Convex Optimization

A set C is **convex** if the line segment between any two points in C lies in C. That is if for any $x_1, x_2 \in C$ and any θ with $0 \le \theta \le 1$, we have $\theta x_1 + (1 - \theta)x_2 \in C$.

A function $f: \mathbb{R}^n \to \mathbb{R}$ is **convex** if the domain of f is a convex set and if for all x, y in the

domain of f, and θ with $0 \le \theta \le 1$, we have

$$f(\theta x + (1 - \theta)y) \le \theta f(x) + (1 - \theta)f(y). \tag{1.4}$$

A convex optimization problem, therefore, is an optimization problem of the form

minimize
$$f_0(x)$$

subject to $f_i(x) \le 0$, $i = 1, ..., m$ (1.5)
 $a_i^T = b_i$, $i = 1, ..., p$

where f_0, \ldots, f_m are convex functions.

There are three additional requirements that differentiate a convex optimization problem from a general optimization problem:

- the objective function must be convex
- the inequality constraint functions must be convex
- the equality constraint functions must be affine

In a convex optimization problem we minimize a convex objective function over a convex set.

In a convex optimization problem, any locally optimal point is also globally optimal. This is a *very* useful fact!

Why might local optimality implying global optimality be useful? Consider a situation where we have a convex objective function. If we are able to find any minimum value for the objective function, then we know this value is not just a local minimum, but indeed a global minimum. If we do not have a convex function, we cannot be as assured that we have found the global optimal value. For example, consider a function such as the one shown in Figure 1.2. An optimization strategy may find the local minimum near x = 1, but since the function is not convex, we cannot conclude that this value is the truly optimal value. In fact, we see that the global minimum, and hence the actual optimal value, is between x = -1 and x = -0.5. On the other hand, if we have a convex

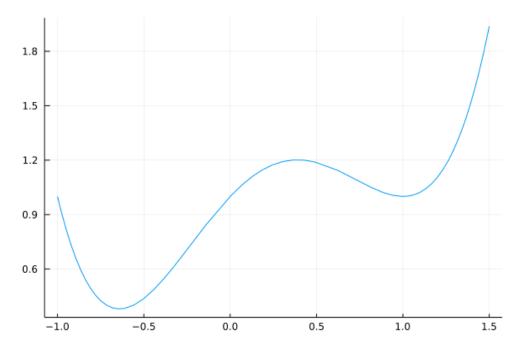


Figure 1.2: A graph of the non-convex function $f(x) = x^4 - x^3 - x^2 + x + 1$. Notice it has two local minima and that the right local minima is not equal to the global minimum.

function, as soon as we find a local minima, we can be assured that it is also the global minima!

So we can see that convexity is a very powerful and useful property in terms of optimization problems. As a result, any time we can take advantage of convexity or approximate functions using convex functions, we often do so.

1.3 Optimization Methods

Chapter 2

SIMP Optimization

- 2.1 The Method of Moving Asymptotes (MMA)
- **2.2** Solid Isotropic Material with Penalization (SIMP)

References

Boyd, S. P. & Vandenberghe, L. (2004). Convex optimization. Cambridge Univ. Pr.

Appendix A

Julia Codes

A.1 Backtracking Line Search

Here is an implementation of the Backtracking Line Search in Julia with default values for the parameters being $\alpha = 0.25$ and $\beta = 0.5$.

```
function ln_srch(d_dir,x,f,fx,dfx;alpha=0.25,beta=0.5)

t = 1

x1 = x+t*d_dir

y1 = f(x1)

y2 = fx+alpha*t*(dfx)'*d_dir

while y1 > y2

t = beta*t

x1 = x+t*d_dir

y1 = f(x1)

y2 = fx+alpha*t*(dfx)'*d_dir

end

return t

end
```

A.2 Gradient Descent

```
using LinearAlgebra
#Function to Optimize
```

```
f(x) = (x[2])^3-x[2]+(x[1])^2-3x[1]
#Gradient of Function
df(x) = [2x[1]-3, 3x[2]^2-1]
#Initial Point
x = [0, 0]
#Gradient Descent Algorithm
function grad_d(f,df,x)
d_dir = -df(x)
t = ln_srch(d_dir, x, f, f(x), df(x))
x = x + t*d_dir
return x
#Compute Minimum for Defined Tolerance
while norm(df(x))>0.00001
global x = grad_d(f,df,x)
end
display(x)
```