USER-INTERACTIVE LEVEL SET IMAGE SEGMENTATION

by

Brady C McCary

APPROVED BY SUPERVISORY COMMITTEE:

Dr. Yan Cao, Chair

Dr. M. Ali Hooshyar

Dr. Mieczyslaw Dabkowski

Dr. Sam Efromovich

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To everyone who has ever written a dedication.

USER-INTERACTIVE LEVEL SET IMAGE SEGMENTATION

by

BRADY C MCCARY, B.S., M.S.

DISSERTATION

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March 2011

PREFACE

This dissertation was produced in accordance with guidelines which permit the inclusion as part of the dissertation the text of an original paper or papers submitted for publication. The dissertation must still conform to all other requirements explained in the Guide for the Preparation of Master's Theses and Doctoral Dissertations at The University of Texas at Dallas. It must include a comprehensive abstract, a full introduction and literature review and an overall conclusion. Additional material (procedural and design data as well as descriptions of equipment) must be provided in sufficient detail to allow a clear and precise judgment to be made of the importance and originality of the research reported.

It is acceptable for this dissertation to include as chapters authentic copies of papers already published, provided these meet type size, margin and legibility requirements. In such cases, connecting texts which provide logical bridges between different manuscripts are mandatory. Where the student is not the sole author of a manuscript, the student is required to make an explicit statement in the introductory material to that manuscript describing the student's contribution to the work and acknowledging the contribution of the other author(s). The signatures of the Supervising Committee which precede all other material in the dissertation attest to the accuracy of this statement.

USER-INTERACTIVE LEVEL SET IMAGE SEGMENTATION

Publication No. _____

Brady C McCary, Ph.D.
The University of Texas at Dallas, 2011

Supervising Professor: Dr. Yan Cao

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CHAPTER 1

INTRODUCTION TO LOREM IPSUM

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1.2 Blah

The general technique for using level set methods in image segmentation is as follows. First, construct a functional F on the space of level set functions. This functional should be such that local minimizers are desired segmentations. A particularly common and fortunate form

of functional is

$$F(\psi) = \int_\Omega G(\psi)\, dx.$$

Next, we find the Euler-Lagrange equation corresponding to F which is a necessary condition for the minimizers of F. For example, when F is of the preceeding form, then we can compute the Euler-Lagrange equations as follows. First, compute the Gâteaux variation of F.

$$\begin{aligned}
0 &= \partial_\psi^h F \\
&= \frac{\partial}{\partial \varepsilon}\Big(F(\psi + \varepsilon h)\Big)\Big|_{\varepsilon=0} \\
&= \frac{\partial}{\partial \varepsilon}\left(\int_\Omega G(\psi + \varepsilon h)\, dx\right)\Bigg|_{\varepsilon=0} \\
&= \int_\Omega \frac{\partial}{\partial \varepsilon}\Big(G(\psi + \varepsilon h)\Big)\Big|_{\varepsilon=0}\, dx \\
&= \int_\Omega \langle \mathrm{D}_\psi\, G, h\rangle\ dx. \qquad (1.1)
\end{aligned}$$

Here, $\mathrm{D}_\psi\, G$ denotes the Fréchet derivative of G evaluated at ψ. We have included several steps in order to illustrate some of the assumptions being made (for example, that the derivative and the integral commute). We require Equation (1.1) to be true for arbitrary h, a necessary condition for ψ to be an optimal point. This implies that $\mathrm{D}_\psi\, G = 0$, which is the Euler-Lagrange equation corresponding to the functional F. Given an initial condition ψ_0, we can proceed to a local minimum by the following gradient descent.

$$\frac{\partial \psi}{\partial t} + \mathrm{D}_\psi\, G = 0$$

For certain functionals F this gradient descent is already a level set equation. However, in some cases it may be necessary to modify this equation by rescaling ψ without moving

the zero level set $\{\psi = 0\}$. This rescaling is justified because the level set method is only tracking the zero level set anyway. Typical rescalings include the following.

$$\frac{\partial \psi}{\partial t} + \delta(\psi)\, \mathrm{D}_\psi\, G = 0$$
$$\frac{\partial \psi}{\partial t} + \mathrm{D}_\psi\, G \|\nabla \psi\| = 0$$

In all cases in this report, the gradients computed from functionals are either *curvature* or *propagation* terms in the level set equation, or they are rescaled to be interpeted in this way. In Chapter **??** we consider several image segmentation functionals and their first-order variations. In Chapter **??** we use these ideas to construct a functional on level set functions which includes user input terms. This functional is then minimized using level set methods by the gradient descent described in this section.

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Region Number	Sign			Bit		
	ψ_0	ψ_1	ψ_2	b_0^i	b_1^i	b_2^i
$i = 0$	$+$	$+$	$+$	0	0	0
$i = 1$	$-$	$+$	$+$	1	0	0
$i = 2$	$+$	$-$	$+$	0	1	0
$i = 3$	$-$	$-$	$+$	1	1	0
$i = 4$	$+$	$+$	$-$	0	0	1
$i = 5$	$-$	$+$	$-$	1	0	1
$i = 6$	$+$	$-$	$-$	0	1	1
$i = 7$	$-$	$-$	$-$	1	1	1

CHAPTER 2

INTRODUCTION TO LOREM IPSUM

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2.2 Blah

The general technique for using level set methods in image segmentation is as follows. First, construct a functional F on the space of level set functions. This functional should be such that local minimizers are desired segmentations. A particularly common and fortunate form

of functional is

$$F(\psi) = \int_\Omega G(\psi)\, dx.$$

Next, we find the Euler-Lagrange equation corresponding to F which is a necessary condition for the minimizers of F. For example, when F is of the preceeding form, then we can compute the Euler-Lagrange equations as follows. First, compute the Gâteaux variation of F.

$$\begin{aligned}
0 &= \partial_\psi^h F \\
&= \frac{\partial}{\partial \varepsilon}\Big(F(\psi + \varepsilon h)\Big)\Big|_{\varepsilon=0} \\
&= \frac{\partial}{\partial \varepsilon}\left(\int_\Omega G(\psi + \varepsilon h)\, dx\right)\Bigg|_{\varepsilon=0} \\
&= \int_\Omega \frac{\partial}{\partial \varepsilon}\Big(G(\psi + \varepsilon h)\Big)\Big|_{\varepsilon=0}\, dx \\
&= \int_\Omega \langle \mathrm{D}_\psi\, G, h\rangle\ dx. \qquad (2.1)
\end{aligned}$$

Here, $\mathrm{D}_\psi\, G$ denotes the Fréchet derivative of G evaluated at ψ. We have included several steps in order to illustrate some of the assumptions being made (for example, that the derivative and the integral commute). We require Equation (2.1) to be true for arbitrary h, a necessary condition for ψ to be an optimal point. This implies that $\mathrm{D}_\psi\, G = 0$, which is the Euler-Lagrange equation corresponding to the functional F. Given an initial condition ψ_0, we can proceed to a local minimum by the following gradient descent.

$$\frac{\partial \psi}{\partial t} + \mathrm{D}_\psi\, G = 0$$

For certain functionals F this gradient descent is already a level set equation. However, in some cases it may be necessary to modify this equation by rescaling ψ without moving

the zero level set $\{\psi = 0\}$. This rescaling is justified because the level set method is only tracking the zero level set anyway. Typical rescalings include the following.

$$\frac{\partial \psi}{\partial t} + \delta(\psi)\, \mathrm{D}_\psi\, G = 0$$
$$\frac{\partial \psi}{\partial t} + \mathrm{D}_\psi\, G \|\nabla \psi\| = 0$$

In all cases in this report, the gradients computed from functionals are either *curvature* or *propagation* terms in the level set equation, or they are rescaled to be interpeted in this way. In Chapter **??** we consider several image segmentation functionals and their first-order variations. In Chapter **??** we use these ideas to construct a functional on level set functions which includes user input terms. This functional is then minimized using level set methods by the gradient descent described in this section.

Table 2.1. A table of inscrutable data, so it was made attractive to keep you from considering the data closely. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Donec fermentum urna in elit mollis tempus. Etiam sit amet dolor sit amet odio hendrerit auctor.

Region Number	Sign			Bit		
	ψ_0	ψ_1	ψ_2	b_0^i	b_1^i	b_2^i
$i = 0$	$+$	$+$	$+$	0	0	0
$i = 1$	$-$	$+$	$+$	1	0	0
$i = 2$	$+$	$-$	$+$	0	1	0
$i = 3$	$-$	$-$	$+$	1	1	0
$i = 4$	$+$	$+$	$-$	0	0	1
$i = 5$	$-$	$+$	$-$	1	0	1
$i = 6$	$+$	$-$	$-$	0	1	1
$i = 7$	$-$	$-$	$-$	1	1	1

APPENDIX A

NOTATION, CONVENTIONS, AND PHILOSOPHY

A.1 Notation and Conventions

In mathematical literature it is often preferable to have an abstract representation (e.g., *basis-free*) because such representations are more general. Perhaps just as useful is that abstract representations often lend themselves to a concise notation. In the words of [Munkres, 1991, p. 60], "The usefulness of well-chosen notation can hardly be overemphasized." The main ideas presented in this report use mathematics as an *applied* science with special attention given to computation. In order to translate abstract mathematical models into numerical procedures one must carefully consider the many possible concrete representations and trace the consequences of each decision. Therefore, we add slightly to this quote: The usefullness of a well-chosen and consistent notation can hardly be overemphasized.

For example, let $f : \mathbb{R}^d \to \mathbb{R}$. In the abstract setting, one does not often speak of $x \in \mathbb{R}^d$ as being a *row*-vector or a *column*-vector. One often desires to speak of the gradient of f, denoted ∇f, which is a function $\nabla f : \mathbb{R}^d \to \mathbb{R}^d$. As a matter of convenience, mathematicians often choose to arrange matters so that expressions such as

$$x + (\nabla f)(x) \tag{A.1}$$

make sense. The reasoning is because expressions of the form in Equation B.1 are used in gradient descent. We adopt this choice, and as a practical consequence this means that when we choose a basis for $\mathbb{R}^d$ we require that $x \in \mathbb{R}^d$ and $(\nabla f)(x)$ are both *row*-vectors or both

column-vectors. However, we emphasize that ∇f is *not* the derivative of f. To be precise, let us import the standard definition of derivative for this type of function.

Definition A.1.1 (Differentiability)**.** *Let $\Omega \subset \mathbb{R}^m$ and let $f : \Omega \to \mathbb{R}^n$. Suppose Ω contains an open neighborhood of the point $x \in \Omega$. Then f is said to be* differentiable *at $x \in \Omega$ if there exists a linear function $T_x : \mathbb{R}^m \to \mathbb{R}^n$ such that*

$$\lim_{\|h\| \to 0} \frac{\|f(x+h) - f(x) - T_x(h)\|}{\|h\|} = 0.$$

It is a standard result that if T_x in definition Definition B.1.1 exists then it is unique. In this case T_x referred to as *the derivative of f at x* and is denoted as $\mathrm{D}_x f$. If f is such that $\mathrm{D}_x f$ exists for all $x \in \Omega$, we often speak of the function $\mathrm{D} f : \Omega \to \mathbb{R}^n$ and drop the x subscript.

So let us consider the situation where $f : \mathbb{R}^d \to \mathbb{R}$ and $\mathrm{D}_x f$ is defined for all $x \in \Omega$. We now present the following question: are $\mathrm{D} f$ and ∇f the same function on Ω? In a certain sense they *are* the same function. However, let us consider what happens if we choose a basis. Let $x \in \mathbb{R}^d$ be fixed and represented as a *column*-vector. This choice is so that T_x may be represented as a matrix which multiplies on the left

$$T_x(h) = T_x h.$$

For $f : \mathbb{R}^d \to \mathbb{R}$ this means that $\mathrm{D}_x f = T_x$ is a *row*-vector so that

$$(\nabla f)(x) = (\mathrm{D}_x f)^{\mathrm{T}}, \tag{A.2}$$

that is, the gradient is the tranpose of the derivative. This fact may be of little import in an abstract setting. In this report, however, we are interested in the implementation of numerical procedures so that bases will be chosen and transpositions must be respected.

The matter is further complicated by the chain rule. Let $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}^d$. In this context, we can compose f and g and if g is a *diffeomporphism* on an open set $\Omega \in \mathbb{R}^d$, then g may be thought of as a change-of-coordinates for f on Ω. Let composition of f with g be denoted $f \circ g$. Then the derivative of $f \circ g$ at $x \in \Omega$ according to the Fréchet rules is

$$\mathrm{D}_x(f \circ g) = (\mathrm{D}_{g(x)}\, f) \circ (\mathrm{D}_x\, g).$$

However, when a basis is chosen one likes to think of $\mathrm{D}_x\, g$ as the Jacobian matrix of g and one likes to think of $\mathrm{D}_{g(x)}\, f$ as $(\nabla f)(g(x))$. The reason is because one might like to have a matrix-vector-product expression of the form

$$(\mathrm{J}\, g) \cdot (\nabla f),$$

where $\mathrm{J}\, g$ is the "Jacobian" of g and ∇f is the column vector of partial derivatives of f. In order for this to be the case, it is necessary that $\mathrm{J}\, g = (\mathrm{D}\, g)^{\mathrm{T}}$. To further complicate matters, other authors form matrix-vector-product expressions of the form

$$(\mathrm{J}\, g)^{\mathrm{T}} \cdot (\nabla f)$$

necessistating that $\mathrm{J}\, g = \mathrm{D}\, g$. Therefore when reading literature with derivatives of this type it is crucial to be aware of what notations and conventions are being used. In some works a basis is assumed, but not mentioned. In other works it assumed that $x + y$ is defined as long as x and y are vectors with the same number of elements, but it does not matter if x is a *row*-vector and y is a *column*-vector. In still other works it is assumed that (in an abuse of

notation) $\mathrm{D} = \nabla$ instead of $\mathrm{D} = \nabla^{\mathrm{T}}$ or that $\mathrm{D} = \mathrm{J}$ instead of $\mathrm{D} = \mathrm{J}^{\mathrm{T}}$. Worst of all is when convention switches between sections.

We have a view to avoid this situation. With this in mind, we take the following conventions in this report. Let us assume we will choose a basis for $x \in \mathbb{R}^d$.

1. $x \in \mathbb{R}^d$ is a *column*-vector.

2. The composition of functions f and g is denoted $f \circ g$. The derivative of $f \circ g$ evaluated at x is

$$\mathrm{D}_x(f \circ g) = (\mathrm{D}_{g(x)}\, f) \circ (\mathrm{D}_x\, g),$$

and when a basis must be chosen this means

$$\mathrm{D}_x(f \circ g) = (\mathrm{D}_{g(x)}\, f)(\mathrm{D}_x\, g).$$

where $\mathrm{D}_{g(x)}\, f$ and $\mathrm{D}_x\, g$ are matrices corresponding to the linear function mentioned in Definition B.1.1.

3. In the special case when $f : \mathbb{R}^d \to \mathbb{R}$, we will enforce the requirement demonstrated in Equation B.2. That is, $\mathrm{D}\, f$ will be a *row*-vector and ∇f is the transpose of $\mathrm{D}\, f$. Written as a matrix,

$$\mathrm{D}\, f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \dots & \frac{\partial f}{\partial x_d} \end{bmatrix} \text{ where } x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}.$$

4. In the case when $g : \mathbb{R}^d \to \mathbb{R}^d$, we will enforce the requirement that the Jacobian of g is the transpose of the derivative of g. That is, $\mathrm{J}\, g = (\mathrm{D}\, g)^{\mathrm{T}}$. Written as a matrix, the

derivative is

$$\mathrm{D}\, g = \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \cdots & \frac{\partial g_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial g_d}{\partial x_1} & \cdots & \frac{\partial g_d}{\partial x_d} \end{bmatrix} \text{ where } x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \text{ and } g = \begin{bmatrix} g_1 \\ \vdots \\ g_d \end{bmatrix}.$$

Besides the finite-dimensional derivatives above, there will be occasion in this report to compute functional derivatives. For completeness, we illustrate the definitions and notation we will use here.

Definition A.1.2 (Fréchet Differentiability)**.** *Let X and Y be Banach spaces and let $Z \subset X$ be open. Then $f : Z \to Y$ is said to be* Fréchet differentiable *at $x \in Z$ if there exists a bounded, linear operator $T_x : Z \to Y$ such that*

$$\lim_{h \to 0} \frac{\|[f(x+h) - f(x)] - T_x(h)\|_Y}{\|h\|_X} = 0.$$

When T_x in Definition B.1.2 exists it is called the Fréchet derivative of f at x and is denoted $\mathrm{D}_x f$. We note that Definition B.1.1 is subsumed in Definition B.1.2. Another useful notion of derivative is a *directional* derivative. In the case of Banach spaces, this is called the Gâteaux derivative.

Definition A.1.3 (Gâteaux Differentiability)**.** *Let X and Y be Banach spaces, let $Z \subset X$ be open, and let $h \in X$ be nonzero and fixed. Then $f : Z \to Y$ is said to be* Gâteaux differentiable *at $x \in Z$ in the direction h if*

$$\lim_{\varepsilon \to 0} \frac{f(x + \varepsilon h) - f(x)}{\varepsilon}$$

exists in Y.

When the limit in Definition B.1.3 exists it called the Gâteaux derivative of f at x in the direction h and is denoted $\partial_x^h f$. When the Gâteaux derivative exists it can be computed directly as

$$\partial_x^h f = \left[\frac{\partial}{\partial \varepsilon}\Big(f(x+\varepsilon h)\Big)\right]\Bigg|_{\varepsilon=0}. \tag{A.3}$$

We note here that if f is Fréchet differentiable then f is Gâteaux differentiable and the corresponding derivatives agree. The converse is not true in general. In the context of this report, we will in general assume that f is a functional on a real Hilbert space and that the Fréchet and Gâteaux derivatives agree. When this is the case, the two derivatives can be related to each other by the following remark.

Remark A.1.1 (The Relation between the Fréchet and Gâteaux derivatives)**.** *Let H be a real Hilbert space, let $f : H \to \mathbb{R}$ be a functional, let $x \in H$ be fixed, let $h \in H$ be fixed. Assume that $\mathrm{D}_x f$ and $\partial_x^h f$ exist. Then these derivatives are related to each other by*

$$\partial_x^h f = \langle \mathrm{D}_x f, h\rangle_H .$$

In this report, we will use Remark B.1.1 several times to "extract" the Fréchet derivative from the Gâteaux derivative because it is much more expedient to compute the Gâteaux derivative according to Equation B.3 than to attempt to use Definition B.1.2 directly.

A.2 Philosophy

The results in this report are framed as optimization problems. In particular, we will describe a state space and to each admissible state we will assign an energy. Given an initial state we will provide the direction to travel in the state space to obtain a lower energy. Mathematically, each state will correspond to a function and the state space in turn will be a Hilbert space. Therefore the map which assigns an energy to a state will be a functional on a Hilbert space, which allows us to use the derivatives described above. In fact all of our

energy functionals will have the form

$$E = \int L, \tag{A.4}$$

which is interpreted to mean (in a sense) that the energy of a state can be found by integrating its individual parts[1]. From here we use a variational principle[2] which is to search for the form of stationary states, that is, where the derivative of the energy functional is zero[3]. It is at the stationary states where the so-called Euler-Lagrange equation of the system is satisfied, which is a necessary condition for optimality. In the case of Equation B.4, the Euler-Lagrange equation takes the form

$$\mathrm{D}_x L = 0, \tag{A.5}$$

so that the state x is optimal only if Equation B.5 is satisfied. Therefore given any initial state x we may use a gradient descent in an artificial time of the form

$$\frac{\partial x}{\partial t} + \mathrm{D}_x L = 0 \tag{A.6}$$

and evolve until steady.

This framework of choosing a function space, choosing an "energy" functional, computing a functional derivative, and using the result to prescribe the necessary for optimal states is pervasive in mathematical physics. In the context of mathematical physics this argument can be used to estimate the evolution equations for classical mechanics and quantum mechanics alike, and it is pleasing to proceed by analogy in this report on image processing. For

[1]The name L in Equation B.4 is chosen because it is referred to as the *Lagrangian* in classical mechanics.

[2]In other contexts, the term *variational principle* may be replaced by *action principle*, *Maupertuis principle* or *principle of least action*. These terms are not equivalent, but the motivations behind their developments are analogous.

[3]Which is analogous to Fermat's theorem.

example, in classical mechanics a system of particles is usually described as having L equal to kinetic energy minus potential energy

$$L = T - V,$$

for each independent particle. E, in turn is a summation over all particles. Because T and V depend on both time and space the resulting Euler-Lagrange equation turns out to be a differential equation which describes the evolution of particles in both time and space. This estimation of reality was deduced through observation of real world phenomena such as the trajectories of projectiles. When the same technique is used in the context of optimization, the situation is slightly more abstracted because there is not a pre-built and faithful simulator[4] to observe and from which to draw conclusions. Instead, one tries to imagine what optimality means and then tries to mathematically describe a universe in which the rules enforce the optimality condition to exist and always be obtained. After this a faithful simulator must be constructed and then finally one can observe. It is usually only after extensive observation that a conclusion about this creative process can be drawn. For example, in the context of Geometric Active Contours [Kass et al., 1987], [Kichenassamy et al., 1995], [Chan and Vese, 2001] the states correspond to closed curves, there is an energy functional, functional derivative and corresponding gradient. In simulation, this gradient can be seen to trace paths through the space of closed curves. To a mathematician it is tempting to wonder whether these paths are geodesics in the space of closed curves because then it might be possible to exploit the additional structure encoded by the metric induced by the geodesics. In fact, this is precisely what was explored in [Caselles et al., 1995] titled *Geodesic Active Contours* and it was shown that in fact these paths are geodesics. Alas, it was later shown in [Michor and Mumford, 2003] that the metric induced by the

[4]In the case of physical sciences, the *physical universe.*

L^2 inner product is pathological[5]. With the benefit of hindsight and a simulator one can see this pathology manifest itself. In particular, the image segmentation functionals given in [Caselles et al., 1995] require a significant regularization term, without which the curve may evolve in a highly irregular fashion for images which are not simple. Two solutions to this problem occurred more-or-less simultaneously in the literature. One solution was presented in [Sundaramoorthi et al., 2005]. In this paper the authors demonstrate that it is not necessary to use L^2 as the Hilbert space of functions and in many cases it may be beneficial to use a Sobolev space. The inner products in these Sobolev spaces generally take the form

$$\langle f, g \rangle_{L^2} + \lambda \langle f', g' \rangle_{L^2} ,$$

where f' and g' are the derivatives of f and g, respectively. The upshot is that because derivatives are involved in the norms, curves remain more regular during evolution. The authors then go on to show that in the two dimensional case that the Sobolev gradient can be obtained from the L^2 gradient via a convolution. Experimentation generally confirms the authors' claims. Another solution to the problem of irregular evolution in the space of curves was given in [Charpiat et al., 2005]. In this paper the authors first provide a similar argument as presented in [Sundaramoorthi et al., 2005], which is to transform one inner product into another via an operator

$$\langle u, v \rangle_L = \langle Lu, v \rangle_F$$

thereby changing the geometry of the associated Hilbert space of functions. The second argument presented in [Charpiat et al., 2005] is that motion in the space of curves can be decomposed. In particular, any gradient direction can be projected onto the mutually orthogonal subspaces T, R or S which are translations, rotations, and scalings, respectively.

[5] I.e., the distance between any two closed curves is zero.

If ∇f is the gradient and $\nabla f|_T$ represents projection onto T, the effect of using $\nabla f|_T$ in a gradient descent is simply to translate f, which is a highly regular evolution.

The purpose of the previous paragraph is to illustrate that this area of applied mathematics[6] is indeed an applied science and that development of theoretical methods and concrete experimentation go hand-in-hand. Therefore in this report, we will endeavor to make all theoretical and experimental details manifest and to motivate the choices as they are made.

[6]But perhaps not all areas of applied mathematics. Some mathematicians consider functional analysis of any kind (even if a simulation is never mentioned or considered) to be far into "applied" spectrum.

APPENDIX B

NOTATION, CONVENTIONS, AND PHILOSOPHY

B.1 Notation and Conventions

In mathematical literature it is often preferable to have an abstract representation (e.g., *basis-free*) because such representations are more general. Perhaps just as useful is that abstract representations often lend themselves to a concise notation. In the words of [Munkres, 1991, p. 60], "The usefulness of well-chosen notation can hardly be overemphasized." The main ideas presented in this report use mathematics as an *applied* science with special attention given to computation. In order to translate abstract mathematical models into numerical procedures one must carefully consider the many possible concrete representations and trace the consequences of each decision. Therefore, we add slightly to this quote: The usefullness of a well-chosen and consistent notation can hardly be overemphasized.

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$$x + (\nabla f)(x) \tag{B.1}$$

make sense. The reasoning is because expressions of the form in Equation B.1 are used in gradient descent. We adopt this choice, and as a practical consequence this means that when we choose a basis for $\mathbb{R}^d$ we require that $x \in \mathbb{R}^d$ and $(\nabla f)(x)$ are both *row*-vectors or both

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$$\lim_{\|h\| \to 0} \frac{\|f(x+h) - f(x) - T_x(h)\|}{\|h\|} = 0.$$

It is a standard result that if T_x in definition Definition B.1.1 exists then it is unique. In this case T_x referred to as *the derivative of f at x* and is denoted as $\mathrm{D}_x f$. If f is such that $\mathrm{D}_x f$ exists for all $x \in \Omega$, we often speak of the function $\mathrm{D} f : \Omega \to \mathbb{R}^n$ and drop the x subscript.

So let us consider the situation where $f : \mathbb{R}^d \to \mathbb{R}$ and $\mathrm{D}_x f$ is defined for all $x \in \Omega$. We now present the following question: are $\mathrm{D} f$ and ∇f the same function on Ω? In a certain sense they *are* the same function. However, let us consider what happens if we choose a basis. Let $x \in \mathbb{R}^d$ be fixed and represented as a *column*-vector. This choice is so that T_x may be represented as a matrix which multiplies on the left

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The matter is further complicated by the chain rule. Let $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}^d$. In this context, we can compose f and g and if g is a *diffeomporphism* on an open set $\Omega \in \mathbb{R}^d$, then g may be thought of as a change-of-coordinates for f on Ω. Let composition of f with g be denoted $f \circ g$. Then the derivative of $f \circ g$ at $x \in \Omega$ according to the Fréchet rules is

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where $\mathrm{D}_{g(x)}\, f$ and $\mathrm{D}_x\, g$ are matrices corresponding to the linear function mentioned in Definition B.1.1.

3. In the special case when $f : \mathbb{R}^d \to \mathbb{R}$, we will enforce the requirement demonstrated in Equation B.2. That is, $\mathrm{D}\, f$ will be a *row*-vector and ∇f is the transpose of $\mathrm{D}\, f$. Written as a matrix,

$$\mathrm{D}\, f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \dots & \frac{\partial f}{\partial x_d} \end{bmatrix} \text{ where } x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}.$$

4. In the case when $g : \mathbb{R}^d \to \mathbb{R}^d$, we will enforce the requirement that the Jacobian of g is the transpose of the derivative of g. That is, $\mathrm{J}\, g = (\mathrm{D}\, g)^{\mathrm{T}}$. Written as a matrix, the

derivative is

$$\mathrm{D}\, g = \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \cdots & \frac{\partial g_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial g_d}{\partial x_1} & \cdots & \frac{\partial g_d}{\partial x_d} \end{bmatrix} \text{ where } x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \text{ and } g = \begin{bmatrix} g_1 \\ \vdots \\ g_d \end{bmatrix}.$$

Besides the finite-dimensional derivatives above, there will be occasion in this report to compute functional derivatives. For completeness, we illustrate the definitions and notation we will use here.

Definition B.1.2 (Fréchet Differentiability)**.** *Let X and Y be Banach spaces and let $Z \subset X$ be open. Then $f : Z \to Y$ is said to be* Fréchet differentiable *at $x \in Z$ if there exists a bounded, linear operator $T_x : Z \to Y$ such that*

$$\lim_{h \to 0} \frac{\|[f(x+h) - f(x)] - T_x(h)\|_Y}{\|h\|_X} = 0.$$

When T_x in Definition B.1.2 exists it is called the Fréchet derivative of f at x and is denoted $\mathrm{D}_x f$. We note that Definition B.1.1 is subsumed in Definition B.1.2. Another useful notion of derivative is a *directional* derivative. In the case of Banach spaces, this is called the Gâteaux derivative.

Definition B.1.3 (Gâteaux Differentiability)**.** *Let X and Y be Banach spaces, let $Z \subset X$ be open, and let $h \in X$ be nonzero and fixed. Then $f : Z \to Y$ is said to be* Gâteaux differentiable *at $x \in Z$ in the direction h if*

$$\lim_{\varepsilon \to 0} \frac{f(x + \varepsilon h) - f(x)}{\varepsilon}$$

exists in Y.

When the limit in Definition B.1.3 exists it called the Gâteaux derivative of f at x in the direction h and is denoted $\partial_x^h f$. When the Gâteaux derivative exists it can be computed directly as

$$\partial_x^h f = \left[\frac{\partial}{\partial \varepsilon}\Big(f(x+\varepsilon h)\Big)\right]\Bigg|_{\varepsilon=0}. \tag{B.3}$$

We note here that if f is Fréchet differentiable then f is Gâteaux differentiable and the corresponding derivatives agree. The converse is not true in general. In the context of this report, we will in general assume that f is a functional on a real Hilbert space and that the Fréchet and Gâteaux derivatives agree. When this is the case, the two derivatives can be related to each other by the following remark.

Remark B.1.1 (The Relation between the Fréchet and Gâteaux derivatives)**.** *Let H be a real Hilbert space, let $f : H \to \mathbb{R}$ be a functional, let $x \in H$ be fixed, let $h \in H$ be fixed. Assume that $\mathrm{D}_x f$ and $\partial_x^h f$ exist. Then these derivatives are related to each other by*

$$\partial_x^h f = \langle \mathrm{D}_x f, h\rangle_H .$$

In this report, we will use Remark B.1.1 several times to "extract" the Fréchet derivative from the Gâteaux derivative because it is much more expedient to compute the Gâteaux derivative according to Equation B.3 than to attempt to use Definition B.1.2 directly.

B.2 Philosophy

The results in this report are framed as optimization problems. In particular, we will describe a state space and to each admissible state we will assign an energy. Given an initial state we will provide the direction to travel in the state space to obtain a lower energy. Mathematically, each state will correspond to a function and the state space in turn will be a Hilbert space. Therefore the map which assigns an energy to a state will be a functional on a Hilbert space, which allows us to use the derivatives described above. In fact all of our

energy functionals will have the form

$$E = \int L, \tag{B.4}$$

which is interpreted to mean (in a sense) that the energy of a state can be found by integrating its individual parts[1]. From here we use a variational principle[2] which is to search for the form of stationary states, that is, where the derivative of the energy functional is zero[3]. It is at the stationary states where the so-called Euler-Lagrange equation of the system is satisfied, which is a necessary condition for optimality. In the case of Equation B.4, the Euler-Lagrange equation takes the form

$$\mathrm{D}_x L = 0, \tag{B.5}$$

so that the state x is optimal only if Equation B.5 is satisfied. Therefore given any initial state x we may use a gradient descent in an artificial time of the form

$$\frac{\partial x}{\partial t} + \mathrm{D}_x L = 0 \tag{B.6}$$

and evolve until steady.

This framework of choosing a function space, choosing an "energy" functional, computing a functional derivative, and using the result to prescribe the necessary for optimal states is pervasive in mathematical physics. In the context of mathematical physics this argument can be used to estimate the evolution equations for classical mechanics and quantum mechanics alike, and it is pleasing to proceed by analogy in this report on image processing. For

[1]The name L in Equation B.4 is chosen because it is referred to as the *Lagrangian* in classical mechanics.

[2]In other contexts, the term *variational principle* may be replaced by *action principle*, *Maupertuis principle* or *principle of least action*. These terms are not equivalent, but the motivations behind their developments are analogous.

[3]Which is analogous to Fermat's theorem.

example, in classical mechanics a system of particles is usually described as having L equal to kinetic energy minus potential energy

$$L = T - V,$$

for each independent particle. E, in turn is a summation over all particles. Because T and V depend on both time and space the resulting Euler-Lagrange equation turns out to be a differential equation which describes the evolution of particles in both time and space. This estimation of reality was deduced through observation of real world phenomena such as the trajectories of projectiles. When the same technique is used in the context of optimization, the situation is slightly more abstracted because there is not a pre-built and faithful simulator[4] to observe and from which to draw conclusions. Instead, one tries to imagine what optimality means and then tries to mathematically describe a universe in which the rules enforce the optimality condition to exist and always be obtained. After this a faithful simulator must be constructed and then finally one can observe. It is usually only after extensive observation that a conclusion about this creative process can be drawn. For example, in the context of Geometric Active Contours [Kass et al., 1987], [Kichenassamy et al., 1995], [Chan and Vese, 2001] the states correspond to closed curves, there is an energy functional, functional derivative and corresponding gradient. In simulation, this gradient can be seen to trace paths through the space of closed curves. To a mathematician it is tempting to wonder whether these paths are geodesics in the space of closed curves because then it might be possible to exploit the additional structure encoded by the metric induced by the geodesics. In fact, this is precisely what was explored in [Caselles et al., 1995] titled *Geodesic Active Contours* and it was shown that in fact these paths are geodesics. Alas, it was later shown in [Michor and Mumford, 2003] that the metric induced by the

[4]In the case of physical sciences, the *physical universe.*

L^2 inner product is pathological[5]. With the benefit of hindsight and a simulator one can see this pathology manifest itself. In particular, the image segmentation functionals given in [Caselles et al., 1995] require a significant regularization term, without which the curve may evolve in a highly irregular fashion for images which are not simple. Two solutions to this problem occurred more-or-less simultaneously in the literature. One solution was presented in [Sundaramoorthi et al., 2005]. In this paper the authors demonstrate that it is not necessary to use L^2 as the Hilbert space of functions and in many cases it may be beneficial to use a Sobolev space. The inner products in these Sobolev spaces generally take the form

$$\langle f, g \rangle_{L^2} + \lambda \langle f', g' \rangle_{L^2} ,$$

where f' and g' are the derivatives of f and g, respectively. The upshot is that because derivatives are involved in the norms, curves remain more regular during evolution. The authors then go on to show that in the two dimensional case that the Sobolev gradient can be obtained from the L^2 gradient via a convolution. Experimentation generally confirms the authors' claims. Another solution to the problem of irregular evolution in the space of curves was given in [Charpiat et al., 2005]. In this paper the authors first provide a similar argument as presented in [Sundaramoorthi et al., 2005], which is to transform one inner product into another via an operator

$$\langle u, v \rangle_L = \langle Lu, v \rangle_F$$

thereby changing the geometry of the associated Hilbert space of functions. The second argument presented in [Charpiat et al., 2005] is that motion in the space of curves can be decomposed. In particular, any gradient direction can be projected onto the mutually orthogonal subspaces T, R or S which are translations, rotations, and scalings, respectively.

[5] I.e., the distance between any two closed curves is zero.

If ∇f is the gradient and $\nabla f|_T$ represents projection onto T, the effect of using $\nabla f|_T$ in a gradient descent is simply to translate f, which is a highly regular evolution.

The purpose of the previous paragraph is to illustrate that this area of applied mathematics[6] is indeed an applied science and that development of theoretical methods and concrete experimentation go hand-in-hand. Therefore in this report, we will endeavor to make all theoretical and experimental details manifest and to motivate the choices as they are made.

[6]But perhaps not all areas of applied mathematics. Some mathematicians consider functional analysis of any kind (even if a simulation is never mentioned or considered) to be far into "applied" spectrum.

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VITA

Brady C McCary was born in Texas in the Fall of 1982, much to his own surprise. He went to The Colony High School as a high school lower classman and the Texas Academy of Mathematics and Science (TAMS) as a high school upper classman. At TAMS, Brady discovered that he was destined to be a sort of mathematician, owing to the finding that the busy work in other disciplines was more than his customs allowed at that time. Simultaneously, Brady discovered the joy of programming, which significantly increased the amount of effort he exerted at any given time. Most of this effort was spent in avoidance of (otherwise) busy work. These kind of adventures and mannerisms generally lead his friends and family to laugh at quotes like the following.

> Some of you may have met mathematicians
> and wondered how they got that way.
>
> Tom Lehrer

After TAMS, Brady went to Southern Methodist University for one semester before transferring to Texas A&M University (TAMU). Simultaneously, Brady applied and was accepted to the Mathematics Advanced Study Semester program at Penn State University (MASS) and the Research in Industrial Projects for Students program (RIPS) at the Institute for Pure & Applied Mathematics at the University of California, Los Angeles. After making it back to TAMU, Brady participated in a few Summer programs under the National Science Foundation title *Vertical Integration of Research and Education in the Mathematical Sciences* (VIGRE). Eventually, Brady graduated from TAMU with a BS in Applied Mathematics.

After a brief tour in a programming job and being trained as a firefighter, Brady entered graduate school in the PhD program in applied mathematical sciences at the University of Texas at Dallas (UTD). While at UTD, Brady received the Graduate Studies Scholarship (GSS). Brady was a teaching assistant, mostly helping Dr. Frank Allum with calculus I and calculus II. Brady received the teaching assistant of the year award in 2008, and then received the Excellence in Education Fellowship in 2009 and 2010. Brady's first publication was [McCary and Cao, 2010], which was the inspiration for this report. In turn, the contents of this report are being prepared into a manuscript for publication in a journal.

During graduate school, Brady met his wife, got married, moved four times, had a son, and expects a daughter not long after the writing of this report. Brady's latest accomplishment is writing exactly 409 words in third person about himself, ending in a sentence with exactly 224 characters, including whitespace, punctuation and numbers, followed by his permanent address.

Permanent address: Brady C McCary
Mathematical Sciences Department
800 West Campbell Road
Richardson, TX 75080-3021