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The Cover: The cover is an artistic rendering of the α-helix, a regular secondary protein structure, being formed by a ribosome reading a strip of RNA, inscribed with a parametrization of the circular helix. The connection between protein structure, energy minimization, and the calculus of variations is discussed in Irena Papst's article in this issue. The cover was designed by Brianna Smrke and rendered by Irena Papst in Adobe Illustrator.

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From the Editors

Dear Reader,

With the conclusion of this issue, Volume I of the *Waterloo Mathematics Review* comes to a close. When we set out to publish this journal we wanted authors from a variety of schools, papers that would cover a diverse set of topics in mathematics, and ten to fifteen papers in each volume. We are happy to say that we have succeeded in each of these goals. We have authors from not just our home school of Waterloo, but also from Ottawa, Simon Fraser, and McMaster. In fact, both authors featured in this issue are not from Waterloo. Our eleven papers discuss a wide range of mathematics from mathematical biology to algebraic combinatorics. We, the editors, are extremely proud of meeting these goals and want to thank all staff and contributors for their help!

However, the next volume presents challenges for us. The Chair of our editorial board is leaving, and we will certainly miss his guidance and expertise in a variety of areas. Fortunately, we have some highly capable rising staff members. Our newest editor, second year Saifuddin Syed, will begin working with us on Volume II, Issue 1. Our new General Manager is Lisa Pidduck. She will be replacing Richard Zsolt, who we wish all the best for at law school. Our new Circulation Manager is Evan Kinsman. With this talented group, we are highly optimistic for the success of Volume II!

Regards,
Frank Ban
Eeshan Wagh
Editors
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Farewell

Dear Reader,

With the conclusion of the first Volume of the *Review* also comes the conclusion of my editorship. From our humble start with authors only from Waterloo the *Review* has grown to boast a cross-Canada writership. The *Review* joins a host of uniquely Canadian mathematical activity at the undergraduate level. The flagship of these activities is the Canadian Undergraduate Mathematics Conference, held every summer. In addition to this gathering of students from all of Canada there are provincial-scope interuniversity activities in Ontario and Quebec, and plans to form similar organizations in other provinces. To those of you who will be continuing your studies after this year, I encourage you to take full advantage of these opportunities and work to expanding them. They are a part of the Canadian undergraduate mathematics experience that is hard to find elsewhere. To those of you concluding your studies, I hope you will continue to spread mathematics—not only the body of truths and methods, but also the communal aspects—wherever this life my take you.

It has been an extreme pleasure to edit this journal and work with our talented reviewers, authors, and staff. I have no doubt that their excellence will ensure that the *Review* will continue for years to come. I am also happy to welcome Saifuddin Syed to the editorial board. I finally must thank Dr. Ian Goulden, dean of the Faculty, Dr. Frank Zorzitto, our Faculty Adviser, and the students and faculty at Waterloo for their ever present support for the *Review*. Without them this project would not be possible.

Farewell,
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Editor, Chair, Volume I
Editor Emeritus
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Correction

In Volume I, Issue 2, in the introduction to the article "A Combinatorial Approach to Finding Dirichlet Generating Function Identities" the two identities were mis-printed. Elsewhere in the article they are printed correctly. This error has been corrected on the website.

A Biological Application of the Calculus of Variations

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Abstract: In this paper, we introduce the calculus of variations and derive the general Euler-Lagrange equations for functionals that depend on functions of one variable. Although the calculus of variations has traditionally been applied to problems in mechanics, we apply the variational approach to a problem in biology by means of minimal surfaces. We introduce the idea of using space curves to model protein structure and lastly, we analyze the free energy associated with these space curves by deriving two Euler-Lagrange equations dependent on curvature.

1 Introduction to the Calculus of Variations

Problems of the calculus of variations came about long before the method. The first problems can be traced back to isoperimetric problems tackled by the Greeks. One such problem is that of Queen Dido, who desired that a given length of oxhide strips enclose a maximum area. This problem, as with many other isoperimetric problems, was solved using geometric methods and reasoning [AB]. However, the first problem solved using some form of the calculus of variations was the problem of the passage of light from one medium to another, and was resolved by Fermat.

In simplest terms, the calculus of variations can be compared to one-dimensional, standard calculus; that is, the study of a function $y = f(x)$ in one variable, for $x \in \mathbb{R}$. Suppose $y = f(x)$ is of class C^1, meaning continuous and differentiable in its domain, which we take to be $x \in \mathbb{R}$. We can seek the local and global extrema of the function, which potentially occur at some $x_i \in \mathbb{R}$, by studying the first and second derivatives. Similarly, the calculus of variations is the study of a functional of the form

$$E[y] = \int_a^b F(t, y(t), y'(t))\, dt, \tag{1.1}$$

where the integrand $F(t, y(t), y'(t))$ is a function of the independent variable t, a function $y(t)$ and the first derivative $y'(t)$, with prime notation denoting the derivative with respect to t. The function $y(t)$ is in D, the space of all C^1 functions defined on the interval $[a, b]$ with $y(a) = A$ and $y(b) = B$ for any $y(t) \in D$. We can seek the local and global extrema of this functional, which occur potentially at some $y(t) \in D$, by studying the first and second variations. This method is the typical application of the calculus of variations—seeking an unknown optimizer of a property by means of a known functional describing this property. What is interesting in our application to modeling protein structure is that we have known solutions and an unknown energy functional. We apply the calculus of variations to understand this unknown energy functional.

1.1 The First Variation

Consider a known local extrema $y(t)$ of the functional in Equation 1.1. We can perturb this extrema by considering

$$\tilde{y}(t) = y(t) + \epsilon\varphi(t),$$

where ϵ is a small real parameter and $\varphi(t)$ is in $\tilde{D}$, which is the space of all C^1 functions defined on $[a, b]$, with the condition

$$\varphi(a) = \varphi(b) = 0 \tag{1.2}$$

to ensure that the function $\tilde{y}(t)$ remains in the domain space D by preserving the boundary conditions. Suppose $y(t)$ is not only a known local extrema, but a known local minimum. Then,

$$E[y] \leq E[\tilde{y}]$$

for a "close" $\tilde{y}(t)$, meaning $\tilde{y}(t)$ that does not perturb $y(t)$ too much, or $\tilde{y}(t)$ with small $|\epsilon|$. This minimality condition can also be expressed as

$$E[y] \leq E[y + \epsilon\varphi].$$

We note that in the above condition, equality, and therefore a minimum, occurs when $\epsilon = 0$. Consider the first variation, defined as

$$\delta E[\tilde{y}] = \frac{d}{d\epsilon} E[y + \epsilon\varphi] \bigg|_{\epsilon=0}.$$

Recall that in the case of one-dimensional, standard calculus, if $y = f(x)$ is minimized at $x = x_0$, then $\frac{d}{dx} y(x)\big|_{x=x_0} = 0$. So if we think of $E[y + \epsilon\varphi]$ as a function of ϵ, that is a function of one variable, it is minimized at $\epsilon = 0$ and

$$\delta E[\tilde{y}] := \frac{d}{d\epsilon} E[y + \epsilon\varphi] \bigg|_{\epsilon=0} = 0. \tag{1.3}$$

Remark 1.1: In fact, $\delta E[\tilde{y}] = 0$ for all perturbed extrema $\tilde{y}$ in the domain space D. However, it is important to note that, although an extrema implies a vanishing first variation, a vanishing first variation does not imply an extrema; it could simply indicate the analogue of a point of inflection from one-dimensional calculus, in D. Whether or not a function $y(t) \in D$ is a true extrema lies in the study of the second variation, which is again very similar to one-dimensional, standard calculus, where we appeal to the second derivative to discriminate between true extrema and points of inflection. It is very important to be able to distinguish between the two cases, as applications of the calculus of variations often call for an extrema $y(t)$ of the functional in question, under the assumption that $\delta E[\tilde{y}] = 0$, allowing for potential solutions to be derived. These are only potential solutions and not true extrema until the second variation is studied. For a detailed and rigorous discussion of the second variation, see the book by Giaquinta and Hildebrandt [GH96]. For our purposes we will simplify and disregard the second variation.

1.2 Euler-Lagrange Equation

Keeping in mind that y, φ, y' and φ' are functions of t, we can rewrite Equation 1.3 as

$$\delta E[\tilde{y}] = \frac{d}{d\epsilon} \int_a^b F(t, y + \epsilon\varphi, y' + \epsilon\varphi')\, dt \bigg|_{\epsilon=0} = 0.$$

By Leibniz's Rule, the above simplifies to

$$\int_a^b \frac{\partial}{\partial\epsilon} F(t, y + \epsilon\varphi, y' + \epsilon\varphi')\, dt \bigg|_{\epsilon=0} = 0.$$

Applying the chain rule, simplifying and subsequently evaluating at $\epsilon = 0$, we get

$$\int_a^b \frac{\partial F}{\partial t}\frac{dt}{d\epsilon} + \frac{\partial F}{\partial[y+\epsilon\varphi]}\frac{d[y+\epsilon\varphi]}{d\epsilon} + \frac{\partial F}{\partial[y'+\epsilon\varphi']}\frac{d[y'+\epsilon\varphi']}{d\epsilon}\ dt\,\Bigg|_{\epsilon=0} = 0$$

$$\int_a^b \frac{\partial F}{\partial[y+\epsilon\varphi]}\varphi + \frac{\partial F}{\partial[y'+\epsilon\varphi']}\varphi'\ dt\,\Bigg|_{\epsilon=0} = 0$$

$$\int_a^b \frac{\partial F}{\partial y}\varphi + \frac{\partial F}{\partial y'}\varphi'\ dt = 0.$$

Next, we integrate the second term in the above by parts to get

$$\int_a^b \frac{\partial F}{\partial y}\varphi + \frac{\partial F}{\partial y'}\varphi\,\Bigg|_a^b - \int_a^b \frac{d}{dt}\frac{\partial F}{\partial y'}\varphi\ dt = 0,$$

but by Condition 1.2, the middle term vanishes and we are left with

$$\int_a^b \frac{\partial F}{\partial y}\varphi - \frac{d}{dt}\frac{\partial F}{\partial y'}\varphi\ dt = 0,$$

which can be written as

$$\int_a^b \left[\frac{\partial F}{\partial y} - \frac{d}{dt}\frac{\partial F}{\partial y'}\right]\varphi\ dt = 0. \tag{1.4}$$

Next, we apply the Fundamental Lemma of the Calculus of Variations.

Lemma 1.1 (Fundamental Lemma of the Calculus of Variations). Let $f(x)$ be a function of class C^n, that is, n-times continuously differentiable, on the interval $[a,b]$. Assume

$$\int_a^b f(x)g(x)\ dx = 0 \tag{1.5}$$

holds for any C^n function $g(x)$ on $[a,b]$ with $g(a) = g(b) = 0$. Then $f(x)$ is identically zero on $[a,b]$.

Proof. (by contradiction) Assume $f(x)$ is a C^n function on $[a,b]$ and Equation 1.5 holds for any C^n function $g(x)$ on $[a,b]$ with $g(a) = g(b) = 0$. In particular, choose a function $g(x)$ such that $g(x) = f(x) \quad \forall\, x \in (a,b)$. Then, Equation 1.5 reduces to

$$\int_a^b f^2\ dx = 0. \tag{1.6}$$

Assume that $f(x)$ is not identically zero. Without loss of generality, there exists an $x_0 \in [a,b]$ such that $f(x_0) > 0$. Since f(x) is continuous, then there must be some subinterval $[a_i, b_i]$ of $[a,b]$ such that all $x_i \in [a_i, b_i]$ have the property that $f(x_i) > 0$, including $x_i = x_0$. Now we take Equation 1.6 and rewrite it as

$$\int_a^b f^2\ dx = \int_a^{a_i} f^2\ dx + \int_{a_i}^{b_i} f^2\ dx + \int_{b_i}^b f^2\ dx. \tag{1.7}$$

We note that the first and the third terms above are either greater than or equal to zero, due to the fact that their integrands are greater than or equal to zero on their respective intervals. However, the second term is strictly greater than zero since its integrand is strictly greater than zero on the interval (a_i, b_i). Thus, the sum of these three integrals is strictly greater than zero, which contradicts our assumption, Equation 1.6. Therefore, f(x) must be identically zero.

□

Applying the Fundamental Lemma to Equation 1.4, with $f(t) = \frac{\partial F}{\partial y} - \frac{d}{dt}\frac{\partial F}{\partial y'}$ and $g(t) = \varphi$, we conclude that

$$\frac{\partial F}{\partial y} - \frac{d}{dt}\frac{\partial F}{\partial y'} = 0, \tag{1.8}$$

which is the Euler-Lagrange equation associated with the first variation of Equation 1.1.

2 Minimal Surfaces

The intuitive definition of a minimal surface is a surface which minimizes surface area. This definition translates nicely to a problem of the calculus of variations, in which a minimal surface is a surface $S = \{(x, y, z) \in \mathbb{R}^3 \mid z = g(x, y)\}$ that minimizes the surface area functional

$$S[g] = \iint F(x, y, g, g_x, g_y)\, dxdy = \iint \sqrt{1 + g_x^2 + g_y^2}\, dxdy \tag{2.1}$$

among admissible surfaces $z = g(x, y)$. Note that the subscript notation g_x denotes the partial derivative of g with respect to x. The associated Euler-Lagrange equation is

$$\frac{\partial F}{\partial g} - \frac{d}{dx}\frac{\partial F}{\partial g_x} - \frac{d}{dy}\frac{\partial F}{\partial g_y} = 0.$$

Notice that F does not depend explicitly on g, so the above simplifies to

$$\frac{d}{dx}\frac{\partial F}{\partial g_x} + \frac{d}{dy}\frac{\partial F}{\partial g_y} = 0. \tag{2.2}$$

Computing the appropriate partial derivatives, plugging them into Equation 2.2 and simplifying, we get

$$\begin{aligned} \frac{d}{dx}\left[\frac{g_x}{\sqrt{1 + g_x^2 + g_y^2}}\right] + \frac{d}{dy}\left[\frac{g_y}{\sqrt{1 + g_x^2 + g_y^2}}\right] &= 0 \\ \frac{g_{xx}\sqrt{1 + g_x^2 + g_y^2} - g_x\left[\frac{g_x g_{xx} + g_y g_{xy}}{\sqrt{1+g_x^2+g_y^2}}\right] + g_{yy}\sqrt{1 + g_x^2 + g_y^2} - g_y\left[\frac{g_x g_{xy} + g_y g_{yy}}{\sqrt{1+g_x^2+g_y^2}}\right]}{1 + g_x^2 + g_y^2} &= 0 \\ \frac{g_{xx}(1 + g_x^2 + g_y^2) - g_x^2 g_{xx} - g_x g_y g_{xy} + g_{yy}(1 + g_x^2 + g_y^2) - g_x g_y g_{xy} - g_y^2 g_{yy}}{\sqrt{1 + g_x^2 + g_y^2}} &= 0 \\ (1 + g_y^2)g_{xx} - 2g_x g_y g_{xy} + (1 + g_x^2)g_{yy} &= 0, \end{aligned}$$

which is the Minimal Surface Equation for the graph g.

3 Regular Secondary Structures in Proteins

It turns out that there is a rather neat application of minimal surfaces to modeling protein structure.

3.1 An Introduction to Basic Protein Structure

A protein is a chain of amino acids, also called a polypeptide chain, that has some biological function related to its structure. Protein structure can be described on four levels: primary, secondary, tertiary and quaternary structure. The primary structure describes the sequence of amino acids, while the secondary structure describes the way in which small portions of the chain are shaped, or in other words describes the

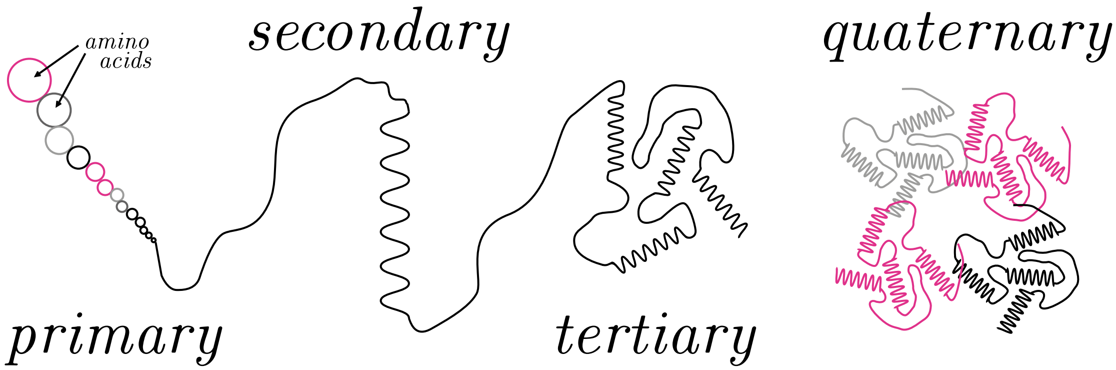

Figure 3.1: A good way to think about protein structure is to imagine zooming out at each step as you move from primary to quaternary.

local structure. The tertiary structure describes how the entire protein chain embeds itself in space and the quaternary structure describes the configuration of multiple polypeptide chains that combine to form one, larger, protein.

We will think of a protein mathematically as a smooth space curve that connects the α-carbons, which is a good approximation of the protein's overall structure as α-carbons form the main backbone. In terms of the application of minimal surfaces, we are interested in one of the most common regular secondary structures: namely, the α-helix, which can be modeled mathematically by a regular helix. Helices are special curves that lie on the surface of a helicoid, a minimal surface.

3.2 The Helicoid

To understand the helicoid, let us consider one parametrization, namely

$$\vec{x}(u,v) = (-b\,\sinh v\,\sin u\,, b\,\sinh v\,\cos u\,, bu) \qquad \left\{ \begin{array}{c} -\infty < u < \infty \\ -\infty < v < \infty \end{array} \right\},$$

where $b \in \mathbb{R}$ is an arbitrary constant. The tangent vectors associated with this parametrization of the helicoid are

$$\begin{aligned} \vec{x}_u &= (-b\,\sinh v\,\cos u\,, -b\,\sinh v\,\sin u\,, b) \\ \vec{x}_v &= (-b\,\cosh v\,\sin u\,, b\,\cosh v\,\cos u\,, 0). \end{aligned}$$

Remark 3.1: The helicoid is the only ruled minimal surface: that is, a surface generated by a family of straight lines. In our parametrization, the generators are $u = c_i$ $(i = 1, ..., n)$, where the c_i are constant.

Notice that our above definition of a minimal surface is not suitable for the helicoid, since we restrict our admissible surfaces to graphs. Instead, to prove that the helicoid is in fact a minimal surface without restricting our domain in the uv-plane to make the helicoid a graph, we will introduce an alternate definition of a minimal surface. However, to understand this definition, we will need to introduce and compute certain quantities that reveal properties of the surfaces' intrinsic geometries. The quantities in question are the coefficients of the first fundamental form.

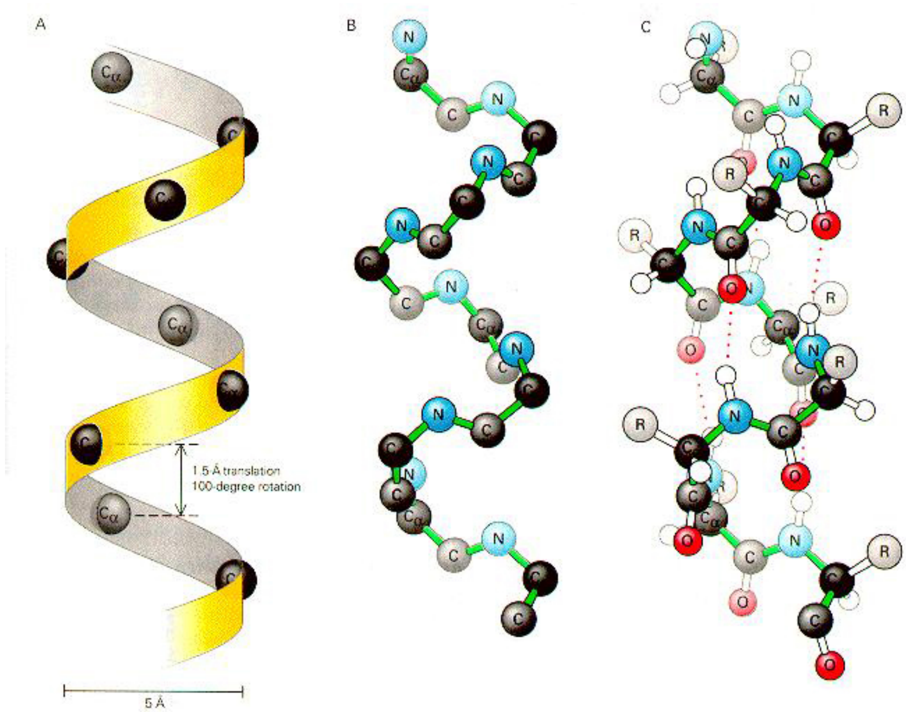

Figure 3.2: The α-helix. Image courtesy of `cmgm.stanford.edu`

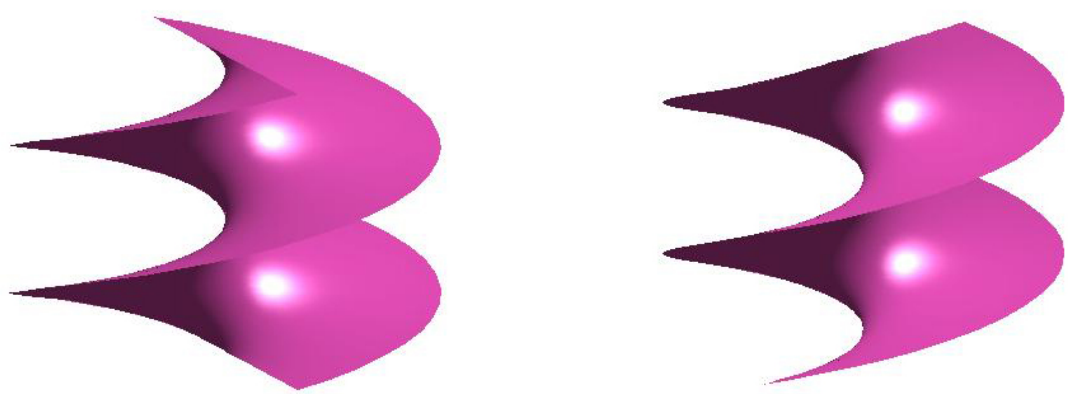

Figure 3.3: The helicoid.

Definition 3.1 (The First Fundamental Form). Let $\vec{x}(u,v) = (x_1(u,v), x_2(u,v), x_3(u,v))$ be a regular parametrized surface in $\mathbb{R}^3$ with tangent vectors

$$\vec{x}_u = \left(\frac{\partial x_1}{\partial u}, \frac{\partial x_2}{\partial u}, \frac{\partial x_3}{\partial u}\right) \qquad \vec{x}_v = \left(\frac{\partial x_1}{\partial v}, \frac{\partial x_2}{\partial v}, \frac{\partial x_3}{\partial v}\right)$$

The *first fundamental form* I of $\vec{x}(u,v)$ is the quadratic form defined by

$$I(du, dv) = \begin{pmatrix} du & dv \end{pmatrix} \begin{pmatrix} E & F \\ F & G \end{pmatrix} \begin{pmatrix} du \\ dv \end{pmatrix},$$

where

$$\begin{aligned} E &= < \vec{x}_u \, , \vec{x}_u > \\ F &= < \vec{x}_u \, , \vec{x}_v > \\ G &= < \vec{x}_v \, , \vec{x}_v > \end{aligned}$$

are the coefficients of the first fundamental form. Note that $< \vec{a} \, , \vec{b} >$ is the Euclidean inner product of $\vec{a}, \vec{b} \in \mathbb{R}^3$.

3.2.1 An Interesting Property of the First Fundamental Form

The *surface area* of a region $\vec{x}(R)$ on $\vec{x}$ is given by

$$A = \iint_R |I|^{\frac{1}{2}} \, dudv.$$

Remark 3.2: Note this property would yield a surface area functional for us to analyze using the calculus of variations. However, computing $|I|^{\frac{1}{2}}$ is fairly involved on its own in this case, and the analysis of the resultant functional would be even more challenging. Instead, we will opt for another, more specific, definition that happens to suit our parametrization of the helicoid quite nicely.

3.2.2 An alternate definition of a minimal surface

The alternate definition of a minimal surface, given in by Louie and Somorjai [LS82], and useful for our purpose, is

Theorem 3.3. Given an isothermally parametrized regular surface $\vec{x}(u,v)$, that is a parametrization with

$$\begin{aligned} E &= G \\ F &= 0 \end{aligned}$$

then $\vec{x}$ is a minimal surface if and only if its coordinate functions are harmonic, that is

$$\vec{x}_{uu} + \vec{x}_{vv} = \vec{0}$$

The coefficients of the first fundamental form associated with our parametrization of the helicoid are

$$\begin{aligned} E = < \vec{x}_u \, , \vec{x}_u > &= b^2 \sinh^2 v \cos^2 u + b^2 \sinh^2 v \sin^2 u + b^2 \\ &= b^2 \sinh^2 v + b^2 \\ &= b^2(\sinh^2 v + 1) \\ &= b^2 \cosh^2 v \\ F = < \vec{x}_u \, , \vec{x}_v > &= b^2 \sinh v \cosh v \sin u \cos u - b^2 \sinh v \cosh v \sin u \, cosu \\ &= 0 \\ G = < \vec{x}_v \, , \vec{x}_v > &= b^2 \cosh^2 v \sin^2 u + b^2 \cosh^2 v \cos^2 u \\ &= b^2 \cosh^2 v. \end{aligned}$$

Note that $E = G$ and $F = 0$.

Now let us show that the isothermally parametrized helicoid has harmonic coordinate functions. Recall the coordinate functions of the helicoid are

$$\vec{x}_{uu} = (b \sinh v \sin u\,, -b \sinh v \cos u\,, 0)$$
$$\vec{x}_{vv} = (-b \sinh v \sin u\,, b \sinh v \cos u\,, 0)$$

which by inspection will sum to zero. Thus, by Theorem 3.3, we conclude that the helicoid is a minimal surface.

3.3 Minimal Surfaces and Protein Structure

Why is it significant that the α-helix, a common regular secondary structure, can be modeled as lying on minimal surfaces? Many minimal surfaces, including the helicoid, occur naturally as a soap film when a wire frame of the surface's boundary is dipped in soap solution.

Figure 3.4: A soap film of a helicoid. Image courtesy of `http://www.math.cornell.edu/~mec/Summer2009/Fok/index.html`

Physically, this phenomenon makes sense as surface area being minimized also minimizes surface tension which is related to potential energy. Equilibrium states, such as that of soap films, often minimize potential energy, and this case is no exception.

In terms of proteins, structure is determined by the non-covalent (non-bonding) forces among and between the amino acids of the polypeptide chain. There are two theories as to why our regular secondary structure of interest should be thought of as lying on a minimal surface. The first theory is that non-polar groups on the polypeptide chain tend to configure themselves in a way that reduces the interface area between themselves and the polar solvent, which is often water in biological systems. Non-polar and polar groups repel each other, so a minimization of the interface surface area is fitting. The other theory is that the minimality could be due to molecular forces that are trying to reduce stress in the regular structures [LS82].

In either case, it makes sense to consider the α-helix as lying on the helicoid. Moreover, the native, or equilibrium, conformation of the entire protein can be thought of as lying on a collection of minimal surfaces connected by turns and random coils that are thought to provide the necessary flexibility for the best energetic configuration of this collection of minimal surfaces.

3.4 Geodesics on Helicoids

Let us take a closer look at helices by considering the parametrization

$$\vec{c}(u) = (-b\sin u, b\cos u, u) \qquad \{-\infty < u < \infty\}$$

It turns out that helices are actually geodesics, or length minimizing curves, on helicoids. According to Louie and Somorjai, the geodesics for the helicoid are given by the differential equations

$$\frac{d^2u}{ds^2} = 0$$

$$\frac{d^2v}{ds^2} + \tanh\left(\frac{dv}{ds}^2 - \frac{du}{ds}^2\right) = 0$$

and solutions to this set of differential equations are

$$\sinh v(s) = A \sinh\left(u(s) + B\right)$$

$$u(s) = Cs + D,$$

where A, B, C and D are constants of integration [LS82]. However, for sufficiently small $|u|$ and $|v|$, the geodesic is approximated by

$$v(s) = A(u(s) + B).$$

So, geodesics on the helicoid are images of straight line segments in the uv-plane. Ignoring any shifting or scaling of this linear function, and taking $v = u$, we see that the parametrization of the helicoid simplifies to

$$\vec{x}(u) = (-b \sinh u \sin u\,, b \sinh u \cos u\,, bu).$$

With sufficiently small $|u|$ and $|v|$, this parametrization is approximated by

$$\vec{x}(u) = (-b\sin u, b\cos u\,, bu),$$

which is a helix. This result makes sense if we consider the fact that geodesics in Euclidean space are linear functions. It is also significant that helices are geodesics on helicoids, and not just arbitrary curves that lie on this surface. They are length minimizing, which could be related to further minimization of energy in the context of protein structure.

4 Euler-Lagrange Equations and Energy Functionals Associated with Helices

4.1 The Setup

As we have seen, variational problems involve a known functional and unknown solutions, which we seek by deriving the Euler-Lagrange equation. However, when we think of regular secondary protein structures, we have known minimizing solutions in the form of helices, and an unknown energy functional. This energy functional would describe the total free energy of the system, the system being the segment of the protein containing the α-helix in solution. This free energy could involve the intra- and inter-molecular forces among and between the amino acids of the protein, as well as the interaction of the protein with the solution.

We seek the Euler-Lagrange equations associated with an unknown energy functional which represents the free energy of the protein segment, in order to better understand this unknown energy functional. We will assume that this energy functional depends only on the curvature of the space curve. This assumption is reasonable since, according to Feoli et al. [FNS05], the infinitesimal twisting associated with torsion in a protein chain does not require much effort and thus only yields small energy differences.

Let γ be a curve $[a,b] \to \mathbb{R}^3$ that is continuous and minimizes the energy functional

$$E(\gamma) = \int_\gamma F(\kappa)\, dL = \int_a^b F(\kappa(s))\, |\, \gamma'(s)\, |\, ds,$$

where $\kappa(s)$ is the curvature of γ, parametrized by the arc length parameter s and given by

$$\kappa(s) = \frac{|\, \gamma' \times \gamma''\, |}{|\, \gamma'\, |^3}.$$

Note that in this section, the prime notation indicated differentiation with respect to s. Now let

$$\tilde{\gamma}(s) = \gamma(s) + \epsilon_1\psi_1(s)\vec{T}(s) + \epsilon_2\psi_2(s)\vec{N}(s) + \epsilon_3\psi_3(s)\vec{B}(s)$$

be the total perturbation of the minimizing curve given by three component perturbations in the tangential $\vec{T}(s)$, normal $\vec{N}(s)$ and binormal $\vec{B}(s)$ directions. Note that $\vec{T}(s)$, $\vec{N}(s)$ and $\vec{B}(s)$ are all unit vectors and together are known as the Frenet frame. Also, ϵ_i are small parameters and $\psi_i(s)$ are smooth, arbitrary functions such that

$$\psi_i(a) = \psi_i(b) = 0 \qquad i = 1, 2, 3. \tag{4.1}$$

We want to consider the variations

$$\frac{\partial}{\partial \epsilon_i} E(\tilde{\gamma}) \bigg|_{\epsilon_1=\epsilon_2=\epsilon_3=0} = 0$$

for each $i = 1, 2, 3$, which correspond to variations in the tangential, normal and binormal directions respectively. We abbreviate $\epsilon_1 = \epsilon_2 = \epsilon_3 = 0$ as $\epsilon_i = 0$. This method should yield a system of three Euler-Lagrange equations. We will disregard the case of

$$\frac{\partial}{\partial \epsilon_1} E(\tilde{\gamma}) \bigg|_{\epsilon_i=0} = 0$$

since this variation simply corresponds to a reparametrization of the curve $\tilde{\gamma}$, as noted by Hill et al. [HMT08]. Let us consider the variations

$$\frac{\partial}{\partial \epsilon_2} E(\tilde{\gamma}) \bigg|_{\epsilon_i=0} = 0 \qquad \text{and} \qquad \frac{\partial}{\partial \epsilon_3} E(\tilde{\gamma}) \bigg|_{\epsilon_i=0} = 0$$

by first looking at the general case of

$$\frac{\partial}{\partial \epsilon_i} E(\tilde{\gamma}) \bigg|_{\epsilon_1=\epsilon_2=\epsilon_3=0} = 0 \qquad i = 2, 3.$$

We simplify to get

$$\begin{aligned}
\frac{\partial}{\partial \epsilon_i} E(\tilde{\gamma}) \bigg|_{\epsilon_i=0} &= \frac{\partial}{\partial \epsilon_i} \int_{\tilde{\gamma}} F(\kappa)\, dL \bigg|_{\epsilon_i=0} \\
&= \frac{\partial}{\partial \epsilon_i} \int_a^b F(\kappa(s))\, |\, \gamma'(s)\, |\, ds \bigg|_{\epsilon_i=0} \\
&= \int_a^b \frac{\partial F}{\partial \kappa} \frac{\partial \kappa}{\partial \epsilon_i}\, |\, \tilde{\gamma}'\, |\, ds \bigg|_{\epsilon_i=0} + \int_a^b F\, \frac{\partial |\, \tilde{\gamma}'\, |}{\partial \epsilon_i}\, ds \bigg|_{\epsilon_i=0},
\end{aligned}$$

but since $|\,\tilde{\gamma}'\,|_{\epsilon_i=0} = |\,\gamma\,| = 1$, the above simplifies to

$$\frac{\partial}{\partial \epsilon_i} E(\tilde{\gamma})\,\Big|_{\epsilon_i=0} = \int_a^b \frac{\partial F}{\partial \kappa}\frac{\partial \kappa}{\partial \epsilon_i}\, ds\,\Big|_{\epsilon_i=0} + \int_a^b F\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}\, ds\,\Big|_{\epsilon_i=0}. \tag{4.2}$$

In order to simplify Equation 4.2, let us isolate and simplify a few quantities before proceeding.

4.1.1 The integrand $\frac{\partial \kappa}{\partial \epsilon_i}$

Since

$$\kappa = \frac{|\,\tilde{\gamma}' \times \tilde{\gamma}''\,|}{|\,\tilde{\gamma}'\,|^3}$$

then

$$\begin{aligned}
\frac{\partial \kappa}{\partial \epsilon_i} &= \frac{\frac{\partial |\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{\partial \epsilon_i}\,|\,\tilde{\gamma}'\,|^3 - 3\,|\,\tilde{\gamma}'\,|^2\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}\,|\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{|\,\tilde{\gamma}'\,|^6} \\
&= \frac{1}{|\,\tilde{\gamma}'\,|^3}\,\frac{\partial |\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{\partial \epsilon_i} - 3\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}\,\frac{|\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{|\,\tilde{\gamma}'\,|^4} \\
\frac{\partial \kappa}{\partial \epsilon_i}\Big|_{\epsilon_i=0} &= \frac{1}{|\,\tilde{\gamma}'\,|^3}\,\frac{\partial |\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{\partial \epsilon_i}\Big|_{\epsilon_i=0} - 3\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}\,\frac{|\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{|\,\tilde{\gamma}'\,|^4}\Big|_{\epsilon_i=0},
\end{aligned} \tag{4.3}$$

but since $|\,\tilde{\gamma}'\,|_{\epsilon_i=0} = |\,\gamma\,| = 1$, Equation 4.3 simplifies to

$$\frac{\partial \kappa}{\partial \epsilon_i}\Big|_{\epsilon_i=0} = \frac{\partial |\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{\partial \epsilon_i}\Big|_{\epsilon_i=0} - 3\,|\,\tilde{\gamma}'\times\tilde{\gamma}''\,|\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}\Big|_{\epsilon_i=0}, \tag{4.4}$$

but

$$|\,\tilde{\gamma}'\times\tilde{\gamma}''\,|^2\Big|_{\epsilon_i=0} = \kappa^2,$$

as computed by Hill et al. [HMT08]. Equation 4.4 then simplifies further to

$$\frac{\partial \kappa}{\partial \epsilon_i}\Big|_{\epsilon_i=0} = \frac{\partial |\,\tilde{\gamma}'\times\tilde{\gamma}''\,|}{\partial \epsilon_i}\Big|_{\epsilon_i=0} - 3\,\kappa\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}\Big|_{\epsilon_i=0}.$$

Omitting the rest of the computations, we note that

$$\frac{\partial \kappa}{\partial \epsilon_2}\Big|_{\epsilon_i=0} = \psi_2'' + (\kappa^2 - \tau^2)\psi_2 \qquad \text{and} \qquad \frac{\partial \kappa}{\partial \epsilon_3}\Big|_{\epsilon_i=0} = 2\tau\psi_3' - \tau'\psi_3, \tag{4.5}$$

which is the same as the result of Hill et al. [HMT08].

4.1.2 The integrand $\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_i}$

We begin with our perturbed space curve

$$\tilde{\gamma} = \gamma + \epsilon_1\psi_1\vec{T} + \epsilon_2\psi_2\vec{N} + \epsilon_3\psi_3\vec{B}.$$

Using the Frenet equations,

$$\vec{T}' = \kappa\vec{N} \qquad \vec{N}' = -\kappa\vec{T} + \tau\vec{B} \qquad \vec{B}' = -\tau\vec{N},$$

we get

$$\tilde{\gamma}' = [1 + \epsilon_1\psi_1' - \epsilon_2\kappa\psi_2]\,\vec{T} + [\epsilon_1\kappa\psi_1 + \epsilon_2\psi_2' - \epsilon_3\tau\psi_3]\,\vec{N} + [\epsilon_2\psi_2\tau + \epsilon_3\psi_3']\,\vec{B}.$$

Noting that $\vec{T}$, $\vec{N}$ and $\vec{B}$ are unit vectors, we are left with

$$|\,\tilde{\gamma}'\,|^2 = [1 + \epsilon_1\psi_1' - \epsilon_2\kappa\psi_2]^2 + [\epsilon_1\kappa\psi_1 + \epsilon_2\psi_2' - \epsilon_3\tau\psi_3]^2 + [\epsilon_2\psi_2\tau + \epsilon_3\psi_3']^2$$

so

$$\left.\frac{\partial|\,\tilde{\gamma}'\,|^2}{\partial\epsilon_2}\right|_{\epsilon_i=0} = -2\kappa\psi_2 \qquad \text{and} \qquad \left.\frac{\partial|\,\tilde{\gamma}'\,|^2}{\partial\epsilon_3}\right|_{\epsilon_i=0} = 0, \tag{4.6}$$

and since

$$\frac{\partial|\,\tilde{\gamma}'\,|}{\partial\epsilon_i} = \frac{1}{2|\,\tilde{\gamma}'\,|}\frac{\partial|\,\tilde{\gamma}'\,|^2}{\partial\epsilon_i}$$

$$\left.\frac{\partial|\,\tilde{\gamma}'\,|}{\partial\epsilon_i}\right|_{\epsilon_i=0} = \frac{1}{2}\left.\frac{\partial|\,\tilde{\gamma}'\,|^2}{\partial\epsilon_i}\right|_{\epsilon_i=0}.$$

Then Equation 4.6 reduces to

$$\left.\frac{\partial|\,\tilde{\gamma}'\,|}{\partial\epsilon_2}\right|_{\epsilon_i=0} = -\kappa\psi_2 \qquad \text{and} \qquad \left.\frac{\partial|\,\tilde{\gamma}'\,|}{\partial\epsilon_3}\right|_{\epsilon_i=0} = 0. \tag{4.7}$$

4.2 Variation in the Normal Direction

With the above quantities calculated, let us return to Equation 4.2 and first consider the variation in the normal direction, which is given by

$$\left.\frac{\partial}{\partial\epsilon_2}E(\tilde{\gamma})\right|_{\epsilon_i=0} = 0$$

$$\left.\int_a^b \frac{\partial F}{\partial\kappa}\frac{\partial\kappa}{\partial\epsilon_2}\,ds\,\right|_{\epsilon_i=0} + \left.\int_a^b F\,\frac{\partial|\,\tilde{\gamma}'\,|}{\partial\epsilon_2}\,ds\,\right|_{\epsilon_i=0} = 0 \tag{4.8}$$

Substituting Equations 4.5 and 4.7 into Equation 4.8 and then simplifying, we get

$$\int_a^b \frac{\partial F}{\partial\kappa}\,[\psi_2'' + (\kappa^2 - \tau^2)\psi_2]\,ds - \int_a^b F\kappa\,\psi_2\,ds = 0$$

$$\int_a^b \frac{\partial F}{\partial\kappa}\,\psi_2''\,ds + \int_a^b \left[(\kappa^2 - \tau^2)\frac{\partial F}{\partial\kappa}\,F\kappa\right]\psi_2\,ds = 0.$$

Now we integrate the first term by parts, recalling the boundary condition Equation 4.1, and simplify to get

$$\left.\frac{\partial F}{\partial\kappa}\,\psi_2'\,\right|_a^b - \int_a^b \frac{d}{ds}\frac{\partial F}{\partial\kappa}\,\psi_2'\,ds + \int_a^b \left[(\kappa^2 - \tau^2)\frac{\partial F}{\partial\kappa}\, - F\kappa\right]\psi_2\,ds = 0$$

$$-\int_a^b \frac{d}{ds}\frac{\partial F}{\partial\kappa}\,\psi_2'\,ds + \int_a^b \left[(\kappa^2 - \tau^2)\frac{\partial F}{\partial\kappa}\, - F\kappa\right]\psi_2\,ds = 0.$$

Again we integrate the first term by parts and simplify to get

$$\left.-\frac{d}{ds}\frac{\partial F}{\partial\kappa}\,\psi_2\,\right|_a^b + \int_a^b \frac{d^2}{ds^2}\frac{\partial F}{\partial\kappa}\,\psi_2\,ds + \int_a^b \left[(\kappa^2 - \tau^2)\frac{\partial F}{\partial\kappa}\, - F\kappa\right]\psi_2\,ds = 0$$

$$\int_a^b \frac{d^2}{ds^2}\frac{\partial F}{\partial\kappa}\,\psi_2\,ds + \int_a^b \left[(\kappa^2 - \tau^2)\frac{\partial F}{\partial\kappa}\, - F\kappa\right]\psi_2\,ds = 0$$

$$\int_a^b \left[\frac{d^2}{ds^2}\frac{\partial F}{\partial\kappa} + (\kappa^2 - \tau^2)\frac{\partial F}{\partial\kappa}\, - F\kappa\right]\psi_2\,ds = 0.$$

Now we apply the Fundamental Lemma of the Calculus of Variations and get

$$\frac{d^2}{ds^2}\frac{\partial F}{\partial \kappa} + (\kappa^2 - \tau^2)\frac{\partial F}{\partial \kappa} - F\kappa = 0, \tag{4.9}$$

which is the Euler-Lagrange equation associated with the component of the total variation in the normal direction.

4.3 Variation in the Binormal Direction

Next, let us consider the variation in the binormal direction, which is given by

$$\frac{\partial}{\partial \epsilon_3} E(\tilde{\gamma})\bigg|_{\epsilon_i=0} = 0$$

$$\int_a^b \frac{\partial F}{\partial \kappa}\frac{\partial \kappa}{\partial \epsilon_3}\, ds\bigg|_{\epsilon_i=0} + \int_a^b F\,\frac{\partial |\,\tilde{\gamma}'\,|}{\partial \epsilon_3}\, ds\bigg|_{\epsilon_i=0} = 0. \tag{4.10}$$

Substituting (4.5) and (4.7) into (4.10) and then simplifying, we get

$$\int_a^b \frac{\partial F}{\partial \kappa}[-2\tau\psi_3' - \tau'\psi_3]\, ds = 0$$

$$2\int_a^b \frac{\partial F}{\partial \kappa}\tau\psi_3'\, ds + \int_a^b \frac{\partial F}{\partial \kappa}\tau'\psi_3\, ds = 0.$$

Integrate the first term by parts, keeping in mind the boundary condition Equation 4.1, and simplify to get

$$2\tau\frac{\partial F}{\partial \kappa}\psi_3\bigg|_a^b - 2\int_a^b \frac{d}{ds}\left(\frac{\partial F}{\partial \kappa}\tau\right)\psi_3\, ds + \int_a^b \frac{\partial F}{\partial \kappa}\tau'\psi_3\, ds = 0$$

$$\int_a^b \left[\frac{\partial F}{\partial \kappa}\tau' - 2\frac{d}{ds}\left(\frac{\partial F}{\partial \kappa}\tau\right)\right]\psi_3\, ds = 0.$$

Finally, by the Fundamental Lemma of the Calculus of Variations, we get

$$\frac{\partial F}{\partial \kappa}\tau' - 2\frac{d}{ds}\left(\frac{\partial F}{\partial \kappa}\tau\right) = 0,$$

which we simplify to get

$$\frac{\partial F}{\partial \kappa}\tau' - 2\left[\frac{d}{ds}\frac{\partial F}{\partial \kappa}\tau + \frac{\partial F}{\partial \kappa}\tau'\right] = 0$$

$$2\frac{d}{ds}\frac{\partial F}{\partial \kappa}\tau + \frac{\partial F}{\partial \kappa}\tau' = 0, \tag{4.11}$$

which is the Euler-Lagrange equation association with the component of the total variation in the binormal direction.

5 Conclusion

We have looked at the basic results of the calculus of variations, namely the simplest Euler-Lagrange equation (Equation 1.8), and have examined the connection to minimal surfaces. In considering minimal surfaces, we saw the link between the helicoid and the α-helix, one of the most common repeating units of protein structure, and then extended this connection to derive two Euler-Lagrange equations (Equation 4.9) and (Equation 4.11) which are related to the potential free energy functionals $E[\gamma] = \int F(\kappa)\, dL$ of protein structure.

We can use these two Euler-Lagrange equations to derive different solutions $F(\kappa)$. For a detailed discussion of some possible solutions, see the article by McCoy [McC08]. Naturally, we would want to restrict ourselves to $F(\kappa)$ that admit helices as minimizing solutions to the energy functional $E[\gamma]$. It would be even more interesting if we were to look at $F(\kappa)$ that admit helices as unique minimizing solutions to $E[\gamma]$. These solutions could shed some light on protein structure from a different angle, which are current avenues of research [BF09, FNS05, HMT08, McC08].

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GRAPHINGS AND UNIMODULARITY

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ABSTRACT: We extend the concept of the law of a finite graph to graphings, which are, in general, infinite graphs whose vertices are equipped with the structure of a probability space. By doing this, we obtain a vast array of new unimodular measures. Furthermore, we work out in full detail a proof of a known result, which states that weak limits preserve unimodularity.

1 INTRODUCTION

This article looks at graphs from the viewpoint of probability theory by defining measures on the space of rooted graphs. We are concerned with approximating such measures using finite graphs. More precisely, every finite graph G gives rise to a probability measure known as the law of G, and approximations are done by means of weak convergence of sequences of laws.

Unimodularity is a property of probability measures, which is known to be preserved under weak limits. Although this result has been stated by Aldous and Lyons [AL07], Schramm [Sch07], and Elek [Ele10], we begin the article by giving a detailed argument. Following that, we expose an abundant source of examples of unimodular measures using graphings, which are graphs whose vertices support the structure of a probability space.

There are several important open questions that are related to unimodularity. The primary question, brought up by David Aldous and Russell Lyons [AL07], is whether every unimodular measure can be approximated by laws of finite graphs. This problem can be decomposed into the following questions:

1. Can the law of a graphing be approximated by laws of finite graphs?
2. Is every unimodular measure the law of a graphing?

Many of the concepts are introduced without examples, and the reader is encouraged to see this author's previous work [Art11] for a more thorough treatment of the basics. However, note that the notation used here is different.

Gábor Elek discusses some of the material in this article as well [Ele07, Ele10], but proceeds in a slightly different direction. In fact, the notation we use mimics his.

To be consistent, note the following set of guidelines regarding notation and convention. All graphs are assumed to be simple and undirected. Throughout the article, assume that X is a compact metric space. Denote by $\mathcal{M}(X)$ the set of probability measures on X, by $\mathbf{C}(X)$ the set of continuous real-valued functions on X, and by $\mathcal{B}(X)$ the Borel σ-algebra on X. From now on, the reader may assume that all of our measures are probability measures.

If d is a metric on X, then $B_d(x,r) = \{y \in X \ : \ d(x,y) \leq r\}$ is the ball around x of radius r. The set $\mathrm{gr}(f) = \{(x, f(x)) \ : \ x \in X\}$ is the graph of a function $f : X \to Y$.

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2 Measures and metrics

We begin by introducing the basic concepts that are used throughout this article.

Definition 2.1. A sequence $(\mu_n)_{n=1}^{\infty}$ of measures on X *converges weakly* to some $\mu \in \mathcal{M}(X)$ if

$$\int f \; d\mu_n \to \int f \; d\mu$$

for all $f \in \mathbf{C}(X)$. The measure μ is known as the *weak limit* of the given sequence.

If $f : X \to Y$ is a measurable function between the measure spaces X and Y, the *pushforward of* μ is the measure $f_*(\mu)$ on Y defined by

$$f_*(\mu)(B) = \mu(f^{-1}(B))$$

for all measurable subsets B of Y.

Proposition 2.1. Let X and Y be compact metric spaces. Suppose that $f : X \to Y$ is a continuous function. If $(\mu_n)_{n=1}^{\infty}$ is a sequence of measures on X that converges weakly to some $\mu \in \mathcal{M}(X)$, then $(f_*(\mu_n))_{n=1}^{\infty}$ converges weakly to $f_*(\mu)$.

Proof. Let $(\mu_n)_{n=1}^{\infty}$ be a sequence of measures on X that converges weakly to μ. Suppose that $g \in \mathbf{C}(Y)$. Then

$$\int g \; df_*(\mu_n) = \int (g \circ f) \; d\mu_n \to \int (g \circ f) \; d\mu = \int g \; df_*(\mu)$$

because the composition $g \circ f$ is continuous. □

Proposition 2.2. Let (X, d) be an ultrametric space. If $r \leq s$ and $B_d(x, r) \cap B_d(y, s)$ is nonempty, then $B_d(x, r) \subseteq B_d(y, s)$.

Proof. Suppose that z lies in the intersection, which means $d(x, z) \leq r$ and $d(y, z) \leq s$. If $w \in B_d(x, r)$, then

$$d(y, w) \leq \max\{d(y, z), d(z, w)\} \leq \max\{d(y, z), d(z, x), d(x, w)\} \leq s$$

because $d(x, w) \leq r$ and d is an ultrametric, and so $w \in B_d(y, s)$. □

Corollary 2.3. A ball of nonzero radius in an ultrametric space (X, d) is closed and open.

Proof. Consider the ball $B = B_d(x, r)$ for some $x \in X$ and r a positive real number. By definition, B is closed. To see that B is open, let $y \in B$. Since $B_d(x, r) \cap B_d(y, r)$ is nonempty, Proposition 2.2 implies that $B_d(x, r) = B_d(y, r)$. Then

$$\{z \in X \; : \; d(y, z) < r\} \subseteq B_d(y, r) = B_d(x, r) = B,$$

and so B is open. □

Lemma 2.1. Let (X, d) be a compact ultrametric space, and let μ be a measure on X. If $f \in \mathbf{C}(X)$ and ε is a positive real number, there is a simple function

$$s_\varepsilon = \sum_{i=1}^{k} a_i \chi_{B_i}$$

for some real numbers a_i and balls B_i such that $\left|\int (f - s_\varepsilon) \; d\mu\right| < \varepsilon$. The function s_ε does not depend on the measure μ.

Proof. Let ε be a positive real number. Since X is compact, the function f is uniformly continuous, which means there is a positive real number δ such that

$$\forall x \in X \ \ \forall y \in X \ \ d(x,y) < \delta \quad \Rightarrow \quad |f(x) - f(y)| < \varepsilon.$$

Furthermore, the set X can be covered by the collection $\{B_d(x,\delta) \ : \ x \in X\}$ of open sets. Using the fact that X is compact, it follows that

$$X = \bigcup_{i=1}^{k} B_d(x_i, \delta)$$

for some $x_i \in X$. This union is disjoint because X is an ultrametric space. Consider the function

$$s_\varepsilon = \sum_{i=1}^{k} f(x_i)\chi_{B_i}$$

where $B_i = B_d(x_i, \delta)$. Following this, if $x \in X$, there is a unique integer i such that $x \in B_d(x_i, \delta)$. Then

$$|f(x) - s_\varepsilon(x)| = |f(x) - f(x_i)| < \varepsilon$$

because $d(x, x_i) < \delta$. Thus $|f(x) - s_\varepsilon(x)| < \varepsilon$ for all $x \in X$. By several properties of integration, we see that

$$\left|\int (f - s_\varepsilon) \ d\mu\right| \leq \int |f - s_\varepsilon| \ d\mu < \varepsilon,$$

as required. □

Theorem 2.4. Let (X, d) be a compact ultrametric space. A sequence $(\mu_n)_{n=1}^{\infty}$ of measures on X converges weakly to $\mu \in \mathcal{M}(X)$ if and only if

$$\forall \varepsilon > 0 \ \ \forall x \in X \ \ \mu_n(B_d(x,\varepsilon)) \to \mu(B_d(x,\varepsilon)).$$

Proof. Let $B = B_d(x, \varepsilon)$ for some $x \in X$ and ε a positive real number. Since X is an ultrametric space, the set B is closed and open by Corollary 2.3, which means the characteristic function χ_B is continuous on X. If μ is the weak limit of $(\mu_n)_{n=1}^{\infty}$, then

$$\mu_n(B) = \int \chi_B \ d\mu_n \to \int \chi_B \ d\mu = \mu(B).$$

Conversely, to see that the sequence $(\mu_n)_{n=1}^{\infty}$ converges weakly to μ, let $f \in \mathbf{C}(X)$, and let ε be a positive real number. By Lemma 2.1, there is a simple function

$$s_\varepsilon = \sum_{i=1}^{k} a_i \chi_{B_i}$$

such that $|\int (f - s_\varepsilon) \ d\mu| < \varepsilon$ and $|\int (f - s_\varepsilon) \ d\mu_n| < \varepsilon$ for all positive integers n. By the hypothesis and the linearity of integration,

$$\int s_\varepsilon \ d\mu_n \to \int s_\varepsilon \ d\mu,$$

so there exists a positive integer N such that

$$\forall n \geq N \quad \left|\int s_\varepsilon \ d\mu_n - \int s_\varepsilon \ d\mu\right| < \varepsilon.$$

Then

$$\left|\int f\ d\mu_n - \int f\ d\mu\right| \leq \left|\int (f - s_\varepsilon)\ d\mu_n\right| + \left|\int s_\varepsilon\ d\mu_n - \int s_\varepsilon\ d\mu\right| + \left|\int (s_\varepsilon - f)\ d\mu\right| < 3\varepsilon$$

for all integers $n \geq N$, and the result follows. □

We end this section with an important result due to Andrei Kolmogorov and Yuri Prokhorov whose proof is omitted, but is available in a book by Patrick Billingsley [Bil99, p. 17].

Theorem 2.5. Let X be a metric space; let μ and μ_n for all positive integers n be measures on $(X, \mathcal{B}(X))$. Suppose that $\mathcal{A} \subseteq \mathcal{B}(X)$ such that

1. $\mathcal{A}$ is closed under finite intersections, and
2. every open subset of X is the union of countably many elements of $\mathcal{A}$.

If $\mu_n(A) \to \mu(A)$ for all $A \in \mathcal{A}$, then $(\mu_n)_{n=1}^{\infty}$ converges weakly to μ.

3 Rooted and birooted graphs

Next we look at some more basic concepts, which are more specific to our purposes. In the remaining sections, we fix a positive integer Δ.

Let G be a graph. Denote by G_x the connected component of G whose vertex set contains x. Define $d_G(x, y)$ to be the length of the shortest path from x to y in G if G is connected. For every $r \in \mathbb{N}$ and $o \in V(G)$, $B_G(o, r)$ is the subgraph of G induced by the set of vertices

$$\{x \in V(G)\ :\ d_{G_o}(o, x) \leq r\},$$

and $N_G(o)$ is the set of vertices that are adjacent to o.

Definition 3.1. A *rooted graph* is a pair (G, o) where G is a graph and $o \in V(G)$; a *birooted graph* is a triple (G, o_1, o_2) where G is a graph, $o_1 \in V(G)$, and $o_2 \in N_G(o_1)$.

Let $\mathbf{Gr}$ be the set of all isomorphism classes $[G, o]$ of countable, connected rooted graphs (G, o) such that $\deg_G(x) \leq \Delta$ for all $x \in V(G)$.

Define the metric $\rho : \mathbf{Gr} \times \mathbf{Gr} \to \mathbb{R}$ as follows:

$$\rho([G, o], [H, p]) = \begin{cases} 0 & \text{if } [G, o] = [H, p], \\ 2^{-r} & \text{otherwise} \end{cases}$$

where $r = \sup\{s \in \mathbb{N}\ :\ [B_G(o, s), o] = [B_H(p, s), p]\}$. Denote by τ the topology induced by the metric ρ. That is, a basis for τ is the collection of balls in the metric space $(\mathbf{Gr}, \rho)$.

Similarly, $\vec{\mathbf{Gr}}$ is the set of all isomorphism classes $[G, o_1, o_2]$ of countable, connected birooted graphs (G, o_1, o_2) such that $\deg_G(x) \leq \Delta$ for all $x \in V(G)$.

An analogous metric $\vec{\rho} : \vec{\mathbf{Gr}} \times \vec{\mathbf{Gr}} \to \mathbb{R}$ is defined by

$$\vec{\rho}([G, o_1, o_2], [H, p_1, p_2]) = \begin{cases} 0 & \text{if } [G, o_1, o_2] = [H, p_1, p_2], \\ 2^{-r} & \text{otherwise} \end{cases}$$

where $r = \sup\{s \in \mathbb{N}\ :\ [B_G(o_1, s), o_1, o_2] = [B_H(p_1, s), p_1, p_2]\}$. Unsurprisingly, the topology induced by $\vec{\rho}$ is denoted by $\vec{\tau}$.

Of course, the reader should not believe that ρ and $\vec{\rho}$ are, in fact, ultrametrics without careful verification. However, rather than restate the arguments here, we refer the reader to this author's previous work [Art11].

Theorem 3.1. The pairs $(\mathbf{Gr}, \rho)$ and $(\vec{\mathbf{Gr}}, \vec{\rho})$ are compact ultrametric spaces.

We now turn our attention to another collection of graphs, this time having no specified root. Let **Graph** be the set of all isomorphism classes of finite graphs G such that $\deg_G(x) \leq \Delta$ for all $x \in V(G)$.

Definition 3.2. A *rooted r-ball* is a rooted graph $[G, o] \in \mathbf{Gr}$ such that $d_G(x, o) \leq r$ for all $x \in V(G)$. The set of rooted r-balls is denoted by U_r. If $G \in \mathbf{Graph}$ and $o \in V(G)$, then $[B_G(o, r), o] \in U_r$ is the *rooted r-ball around o in G*.

A *birooted r-ball* is a birooted graph $[G, o_1, o_2] \in \vec{\mathbf{Gr}}$ such that $[G, o_1] \in U_r$. The set of birooted r-balls is denoted by $\vec{U}_r$.

If $\alpha \in U_r$ and $\vec{\alpha} \in \vec{U}_r$, let

$$T_r(\mathbf{Gr}, \alpha) = \{[G, o] \in \mathbf{Gr} \ : \ [B_G(o, r), o] = \alpha\}$$

and

$$T_r(\vec{\mathbf{Gr}}, \vec{\alpha}) = \{[G, o_1, o_2] \in \vec{\mathbf{Gr}} \ : \ [B_G(o_1, r), o_1, o_2] = \vec{\alpha}\}.$$

The strange notation of the collections above is adopted from papers by Gábor Elek [Ele07, Ele10], although with the addition of a subscript on the T for better clarity.

Following a few technical results, it will be shown that the two collections above are important subsets of $\mathbf{Gr}$ and $\vec{\mathbf{Gr}}$.

Proposition 3.2. Graph isomorphisms are isometries.

Proof. Let $\varphi : G \to H$ be a graph isomorphism for some graphs G and H. If x and y are connected by a shortest path P in G, then $\varphi(x)$ and $\varphi(y)$ are connected by the shortest path $\varphi(P)$, and so

$$d_G(x, y) = |E(P)| = |E(\varphi(P))| = d_H(\varphi(x), \varphi(y)).$$

Hence φ preserves the shortest path metric, meaning it is an isometry. □

Lemma 3.1. If $[G, o]$ and $[H, p]$ are distinct, then

$$[B_G(o, r), o] = [B_H(p, r), p]$$

if and only if

$$\rho([G, o], [H, p]) \leq 2^{-r}.$$

Proof. Let $\rho([G, o], [H, p]) = 2^{-s}$ where

$$s = \sup\{t \in \mathbb{N} \ : \ [B_G(o, t), o] = [B_H(p, t), p]\}.$$

If $[B_G(o, r), o] = [B_H(p, r), p]$, then $r \leq s$, and so $2^{-s} \leq 2^{-r}$. Conversely, assume that $2^{-s} \leq 2^{-r}$. That is, $r \leq s$. By definition, $[B_G(o, s), o] = [B_H(p, s), p]$. Let $\varphi : B_G(o, s) \to B_H(p, s)$ be a graph isomorphism such that $p = \varphi(o)$. Note that $B_G(o, r) \subseteq B_G(o, s)$, and consider the restriction φ' of φ to $B_G(o, r)$. The image of $B_G(o, r)$ under φ' is $B_H(p, r)$ because φ is an isometry. □

Proposition 3.3. The following equalities hold:

$$T_r(\mathbf{Gr}, [B_G(o, r), o]) = B_\rho([G, o], 2^{-r})$$

and

$$T_r(\vec{\mathbf{Gr}}, [B_G(o_1, r), o_1, o_2]) = B_{\vec{\rho}}([G, o_1, o_2], 2^{-r}).$$

Proof. To see that the first equality is true, observe that

$$\begin{aligned}[H,p] \in T_r(\mathbf{Gr}, [B_G(o,r),o]) &\Leftrightarrow [B_H(p,r),p] = [B_G(o,r),o] \\ &\Leftrightarrow \rho([G,o],[H,p]) \le 2^{-r} \\ &\Leftrightarrow [H,p] \in B_\rho([G,o],2^{-r}),\end{aligned}$$

where the second equivalence holds by Lemma 3.1. The proof of the second equality is analogous. □

Corollary 3.4. The collections $\{T_r(\mathbf{Gr},\alpha) \ : \ r \in \mathbb{N} \ ; \ \alpha \in U_r\}$ and $\{T_r(\vec{\mathbf{Gr}},\vec{\alpha}) \ : \ r \in \mathbb{N} \ ; \ \vec{\alpha} \in \vec{U}_r\}$ are bases for the topologies τ and $\vec{\tau}$, respectively.

Proof. Let $\alpha \in U_r$. Since $\alpha = [G,o]$ for some $[G,o] \in \mathbf{Gr}$ and $d_G(x,o) \le r$ for all $x \in V(G)$, it follows that $\alpha = [B_G(o,r),o]$. That is,

$$\begin{aligned}&\{T_r(\mathbf{Gr},\alpha) \ : \ r \in \mathbb{N} \ ; \ \alpha \in U_r\} \\ &\qquad = \{T_r(\mathbf{Gr},[B_G(o,r),o]) \ : \ r \in \mathbb{N} \ ; \ [G,o] \in \mathbf{Gr}\} \\ &\qquad = \{B_\rho([G,o],2^{-r}) \ : \ r \in \mathbb{N} \ ; \ [G,o] \in \mathbf{Gr}\}\end{aligned}$$

where the second equality holds by Proposition 3.3. The same is true for the latter collection. □

Corollary 3.5. The sets $T_r(\mathbf{Gr},\alpha)$ and $T_r(\vec{\mathbf{Gr}},\vec{\alpha})$ are both closed and open in $\mathbf{Gr}$ and $\vec{\mathbf{Gr}}$, respectively.

Proof. Since $\mathbf{Gr}$ and $\vec{\mathbf{Gr}}$ are ultrametric spaces, the result is true by Corollary 2.3. □

Proposition 3.6. The collection

$$\{T_r(\vec{\mathbf{Gr}},\vec{\alpha}) \ : \ r \in \mathbb{N} \ ; \ \vec{\alpha} \in \vec{U}_r\} \cup \{\emptyset\}$$

1. is closed under finite intersections, and
2. every open subset of $\vec{\mathbf{Gr}}$ is a finite union of its elements.

Proof. The result easily follows from Corollary 3.4 and the compactness of $\vec{\mathbf{Gr}}$. □

4 Laws

Definition 4.1. The *law* is a function $\Psi : \mathbf{Graph} \to \mathcal{M}(\mathbf{Gr})$ defined as follows: for every graph $G \in \mathbf{Graph}$,

$$\Psi(G)[G_o,o] = \frac{|\mathrm{Aut}(G)o|}{|V(G)|}$$

if G_o is a connected component of G for some $o \in V(G)$, and $\Psi(G) = 0$ elsewhere. Here $\mathrm{Aut}(G)$ is the group of automorphisms on G, and $\mathrm{Aut}(G)o$ is the *orbit* of the vertex o in G:

$$\mathrm{Aut}(G)o = \{x \in V(G) \ : \ \exists\varphi \in \mathrm{Aut}(G) \ \ \varphi(x) = o\}.$$

The image $\Psi(G)$ of a finite graph $G \in \mathbf{Graph}$ is a probability measure on $\mathbf{Gr}$ called *the law of G*. Usually, we will simply write *the law* when no reference to a specific graph is necessary.

If $\alpha \in U_r$ and $G \in \mathbf{Graph}$, let

$$T_r(G,\alpha) = \{x \in V(G) \ : \ [B_G(x,r),x] = \alpha\}$$

and

$$p_G(\alpha,r) = \frac{|T_r(G,\alpha)|}{|V(G)|}.$$

Using this notation, Gábor Elek [Ele07, Ele10] defines the weak convergence of "laws" in the following way.

Definition 4.2. A graph sequence $(G_n)_{n=1}^{\infty}$ in **Graph** *converges weakly* if there is a measure μ on **Gr** such that

$$p_{G_n}(\alpha, r) \to \mu(T_r(\mathbf{Gr}, \alpha))$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$.

To see that the quotation marks around the word "laws" are not necessary, consider this next pair of results.

Lemma 4.1. Suppose that $G \in$ **Graph**. Then

$$\Psi(G)(T_r(\mathbf{Gr}, \alpha)) = \frac{|T_r(G, \alpha)|}{|V(G)|}$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$.

Proof. If $G \in$ **Graph**, then

$$\Psi(G)(T_r(\mathbf{Gr}, \alpha)) = \int \chi_{T_r(\mathbf{Gr},\alpha)} \, d\Psi(G) = \frac{1}{|V(G)|} \sum_{x \in V(G)} \chi_{T_r(\mathbf{Gr},\alpha)}[G, x] = \frac{|T_r(G, \alpha)|}{|V(G)|}$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$ where the third equality holds because $\chi_{T_r(\mathbf{Gr},\alpha)}[G, o] = 1$ precisely when $\chi_{T_r(G,\alpha)}(o) = 1$ for all $o \in V(G)$. □

Proposition 4.1. Let $G_n \in$ **Graph** for all positive integers n. The sequence of laws $(\Psi(G_n))_{n=1}^{\infty}$ converges weakly if and only if the graph sequence $(G_n)_{n=1}^{\infty}$ does too.

Proof. Suppose that $(\Psi(G_n))_{n=1}^{\infty}$ converges weakly to some measure μ on **Gr**. By Corollary 3.5, $T_r(\mathbf{Gr}, \alpha)$ is closed and open, which means its characteristic function is continuous on **Gr**. Using the definition of weak convergence and Lemma 4.1,

$$\frac{|T_r(G_n, \alpha)|}{|V(G_n)|} = \int \chi_{T_r(\mathbf{Gr},\alpha)} \, d\Psi(G_n) \to \int \chi_{T_r(\mathbf{Gr},\alpha)} \, d\mu = \mu(T_r(\mathbf{Gr}, \alpha)). \qquad (\star)$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$. Hence $(G_n)_{n=1}^{\infty}$ converges weakly.

Conversely, assume that $(G_n)_{n=1}^{\infty}$ converges weakly. Then Equation $(\star)$ holds for all $r \in \mathbb{N}$ and $\alpha \in U_r$. Hence the sequence $(\Psi(G_n))_{n=1}^{\infty}$ converges weakly to μ by Theorem 2.4 and Proposition 3.3. □

5 Unimodularity versus involution invariance

The following section guides the reader to the first of our goals. Namely, a proof that weak limits preserve the concept known as unimodularity. This result was stated by Itai Benjamini and Oded Schramm [BS01, p. 10], but we give a detailed argument.

5.1 Preliminaries

Definition 5.1. A measure μ on **Gr** is *unimodular* if

$$\int \sum_{x \in N_G(o)} f[G, x, o] \, d\mu[G, o] = \int \sum_{x \in N_G(o)} f[G, o, x] \, d\mu[G, o]$$

for all nonnegative real-valued Borel functions f on $\vec{\mathbf{Gr}}$.

Define the function $\iota : \vec{\mathbf{Gr}} \to \vec{\mathbf{Gr}}$ by $\iota[G,x,y] = [G,y,x]$ for all $[G,x,y] \in \vec{\mathbf{Gr}}$. Every Borel subset A of $\vec{\mathbf{Gr}}$ induces a function $f_A : \mathbf{Gr} \to \mathbb{N}$ defined by

$$f_A[G,o] = |\{x \in N_G(o) \ : \ [G,o,x] \in A\}|$$

for all $[G,o] \in \mathbf{Gr}$. Let μ be a measure on $\mathbf{Gr}$. The measure $\vec{\mu}$ on $\vec{\mathbf{Gr}}$ is defined by $\vec{\mu}(A) = \int f_A \, d\mu$ for all Borel subsets A of $\vec{\mathbf{Gr}}$.

Definition 5.2. A measure μ on $\mathbf{Gr}$ is *involution invariant* if $\iota_*(\vec{\mu}) = \vec{\mu}$.

In fact, the concepts of unimodularity and involution invariance are logically equivalent as the following theorem demonstrates. This result seems to be known based on the different, yet equivalent, approaches taken by Elek [Ele07, Ele10], and Aldous and Lyons [AL07], but there is no explicit argument in the literature.

Theorem 5.1. A measure μ on $\mathbf{Gr}$ is unimodular if and only if it is involution invariant.

Proof. Note that

$$\sum_{x \in N_G(o)} \chi_A[G,o,x] = |\{x \in N_G(o) \ : \ [G,o,x] \in A\}| = f_A[G,o]$$

and

$$\sum_{x \in N_G(o)} (\chi_A \circ \iota)[G,o,x] = |\{x \in N_G(o) \ : \ \iota[G,o,x] \in A\}| = f_{\iota(A)}[G,o]$$

for all Borel subsets A of $\vec{\mathbf{Gr}}$. Suppose that μ is unimodular. Then

$$\iota_*(\vec{\mu})(A) = \vec{\mu}(\iota(A)) = \int f_{\iota(A)}[G,o] \ d\mu[G,o] = \int f_A[G,o] \ d\mu[G,o] = \vec{\mu}(A)$$

for all Borel subsets A of $\vec{\mathbf{Gr}}$. Conversely, if $\iota_*(\vec{\mu}) = \vec{\mu}$, then

$$\int \sum_{x \in N_G(o)} \chi_A[G,o,x] \ d\mu[G,o] = \int \sum_{x \in N_G(o)} (\chi_A \circ \iota)[G,o,x] \ d\mu[G,o]$$

for all Borel subsets A of $\vec{\mathbf{Gr}}$. Since this holds for all characteristic functions, it is true for all simple functions, and so for all nonnegative real-valued Borel functions. □

5.2 Weak limits preserve unimodularity

Having defined and reconciled the definitions of unimodularity and involution invariance, it is time to overcome several technical results, and accomplish our first goal.

Lemma 5.1. If $\varphi : (B_G(o,r), o) \to (B_H(p,r), p)$ is a rooted graph isomorphism, then $N_H(p) = \varphi(N_G(o))$.

Proof. If $y \in \varphi(N_G(o))$, then $y = \varphi(x)$ for some $x \in N_G(o)$. Since φ is a graph isomorphism, Proposition 3.2 implies that

$$d_H(y,p) = d_H(\varphi(x), \varphi(o)) = d_G(x,o) = 1,$$

and so $y \in N_H(p)$. Thus $\varphi(N_G(o)) \subseteq N_H(p)$. On the other hand, assume that $y \in N_H(p)$. Since φ is bijective, there is an $x \in V(G)$ such that $y = \varphi(x)$. Furthermore,

$$d_G(x,o) = d_H(\varphi(x), \varphi(o)) = d_H(y,p) = 1,$$

which means $x \in N_G(o)$. □

Proposition 5.2. The function f_A is Lipschitz when $A = T_r(\vec{\mathbf{Gr}}, \vec{\alpha})$. In particular, it is continuous.

Proof. Let $A = T_r(\vec{\mathbf{Gr}}, \vec{\alpha})$. If $\rho([G,o],[H,p]) \leq 2^{-r}$, there is a rooted graph isomorphism $\varphi : (B_G(o,r), o) \to (B_H(p,r), p)$. By Lemma 5.1, $N_H(p) = \varphi(N_G(o))$. Since φ is an isomorphism, it is easy to see that $f_A[H,p] = f_A[G,o]$. On the other hand, assume that $\rho([G,o],[H,p]) > 2^{-r}$. Then

$$|f_A[G,o] - f_A[H,p]| \leq \Delta = \Delta 2^r 2^{-r} < \Delta 2^r \cdot \rho([G,o],[H,p])$$

because $0 \leq f_A \leq \Delta$. Hence f_A is $\Delta 2^r$-Lipschitz, and so it is continuous. □

Lemma 5.2. If $y \in N_G(x)$, then $B_G(y, r-1) \subseteq B_G(x,r)$.

Proof. Suppose that $y \in N_G(x)$ and $z \in B_G(y, r-1)$. Then $d_G(x,y) = 1$ and $d_G(y,z) \leq r-1$, so

$$d_G(x,z) \leq d_G(x,y) + d_G(y,z) = 1 + d_G(y,z) \leq r,$$

which means $z \in B_G(x,r)$. □

Lemma 5.3. If $[B_G(o_1,r), o_1, o_2] = [B_H(p_1,r), p_1, p_2]$, then

$$[B_G(o_2, r-1), o_2, o_1] = [B_H(p_2, r-1), p_2, p_1].$$

Proof. Suppose that $[B_G(o_1,r), o_1, o_2] = [B_H(p_1,r), p_1, p_2]$. There is a graph isomorphism $\varphi : B_G(o_1,r) \to B_H(p_1,r)$. By Lemma 5.2, $B_G(o_2, r-1) \subseteq B_G(o_1,r)$. Let φ' be the restriction of φ to $B_G(o_2, r-1)$. The image of φ' is $B_H(p_2, r-1)$ because φ is an isometry. It follows that $\varphi' : B_G(o_2, r-1) \to B_H(p_2, r-1)$ is a graph isomorphism. Furthermore, $\varphi'(o_1) = \varphi(o_1) = p_1$ and $\varphi'(o_2) = \varphi(o_2) = p_2$. □

Proposition 5.3. The function ι is a continuous involution. In fact, ι is a self-homeomorphism of $\vec{\mathbf{Gr}}$.

Proof. If $[G, o_1, o_2], [H, p_1, p_2] \in \vec{\mathbf{Gr}}$ are distinct, then

$$\vec{\rho}([G, o_1, o_2], [H, p_1, p_2]) = 2^{-r}$$

and $[B_G(o_1,r), o_1, o_2] = [B_H(p_1,r), p_1, p_2]$. By Lemma 5.3,

$$[B_G(o_2, r-1), o_2, o_1] = [B_H(p_2, r-1), p_2, p_1],$$

and so

$$\vec{\rho}(\iota[G, o_1, o_2], \iota[H, p_1, p_2]) = \vec{\rho}([G, o_2, o_1], [H, p_2, p_1]) \leq 2^{-(r-1)} = 2 \cdot 2^{-r}.$$

Hence ι is 2-Lipschitz, and so it is continuous. Furthermore, ι is a self-homeomorphism because it is an involution. □

Proposition 5.4. If $(\mu_n)_{n=1}^{\infty}$ converges weakly to μ, then $(\vec{\mu}_n)_{n=1}^{\infty}$ converges weakly to $\vec{\mu}$.

Proof. By Proposition 3.6 and Theorem 2.5, it suffices to show that

$$\vec{\mu}_n(T_r(\vec{\mathbf{Gr}}, \vec{\alpha})) \to \vec{\mu}(T_r(\vec{\mathbf{Gr}}, \vec{\alpha}))$$

for all $r \in \mathbb{N}$ and $\vec{\alpha} \in \vec{U}_r$. By Proposition 5.2, f_A is continuous when $A = T_r(\vec{\mathbf{Gr}}, \vec{\alpha})$. Then

$$\vec{\mu}_n(A) = \int f_A \; d\mu_n \to \int f_A \; d\mu = \vec{\mu}(A)$$

because $(\mu_n)_{n=1}^{\infty}$ converges weakly to μ. Thus $(\vec{\mu}_n)_{n=1}^{\infty}$ converges weakly to $\vec{\mu}$. □

Finally, we arrive at our first main result. Using the technical propositions stated above, we proceed to demonstrate the following. The idea for the proof of the following theorem is due to a paper by David Aldous and J. Michael Steele [AS03, p. 40].

Theorem 5.5. If $(\mu_n)_{n=1}^{\infty}$ is a sequence of involution invariant measures on **Gr** that converges weakly to a measure μ on **Gr**, then μ is involution invariant.

Proof. For convenience, let $\mu = \lim_{n\to\infty} \mu_n$. By Proposition 5.4, $\vec{\mu} = \lim_{n\to\infty} \vec{\mu}_n$. Using Proposition 5.3 with Proposition 2.1, we see that $\iota_*(\vec{\mu}) = \lim_{n\to\infty} \iota_*(\vec{\mu}_n)$. Since μ_n is involution invariant for all positive integers n, it follows that $\iota_*(\vec{\mu}) = \lim_{n\to\infty} \vec{\mu}_n$, and so $\iota_*(\vec{\mu}) = \vec{\mu}$, which means μ is involution invariant. □

Corollary 5.6. If $(\mu_n)_{n=1}^{\infty}$ is a sequence of unimodular measures on **Gr** that converges weakly to a measure μ on **Gr**, then μ is unimodular.

Proof. This follows immediately by Theorem 5.1. □

6 Graphings

In this section, the primary focus will be on discovering a potentially vast new source of examples of unimodular measures by showing that the law of a graphing is unimodular. Before doing so, the reader needs to know what a graphing is.

6.1 Preliminaries

For the purposes of this article, we will be using Gábor Elek's definition of a graphing [Ele07]. Although, as it is later shown, there is a more general notion.

Definition 6.1. Let μ be a measure on a Borel space X. A *measurable graphing* is a tuple $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ where i_j is a measure-preserving Borel involution of X for each $j \in \{1, 2, \ldots, k\}$.

The measurable graphing $\mathcal{G}$ determines an equivalence relation $\sim_{\mathcal{G}}$ on X defined as follows: $x \sim_{\mathcal{G}} y$ if and only if there is a subset $\{x_1, x_2, \ldots, x_m\} \subseteq X$ such that

1. $x_1 = x$ and $x_m = y$, and
2. for each $i \in \{1, 2, \ldots, m-1\}$, there is a $j \in \{1, 2, \ldots, k\}$ such that $x_{i+1} = i_j(x_i)$

for all $(x, y) \in X \times X$. The *leafgraph* of $\mathcal{G}$ is a graph $\mathcal{L}$ whose vertex set is X, and x is adjacent to y in $\mathcal{L}$ precisely when $y = i_j(x)$ for some $j \in \{1, 2, \ldots, k\}$.

In passing, we mention the following straightforward fact that relates the equivalence relation $\sim_{\mathcal{G}}$ to the leafgraph of $\mathcal{G}$.

Proposition 6.1. If $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ is a measurable graphing, then the equivalence classes of $\sim_{\mathcal{G}}$ are the connected components of $\mathcal{L}$. Specifically, $V(\mathcal{L}_x) = [x]_{\sim_{\mathcal{G}}}$ and $E(\mathcal{L}_x) = \{yz \ : \ \exists j \in \{1, 2, \ldots, k\} \ \ i_j(y) = z\}$ for all $x \in X$.

Next we define the law of a graphing, which is similar to the law of a finite graph seen previously.

Definition 6.2. Let $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ be a measurable graphing. Denote by $\mathcal{L}$ the leafgraph of $\mathcal{G}$. The *law of* $\mathcal{G}$ is the probability measure $\Psi(\mathcal{G})$ on **Gr** defined by

$$\Psi(\mathcal{G})(T_r(\mathbf{Gr}, \alpha)) = \mu(\{x \in X \ : \ [B_{\mathcal{L}}(x, r), x] = \alpha\})$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$.

By writing $\Psi(\mathcal{L})$ instead of $\Psi(\mathcal{G})$, this definition of a law expands the domain of the function Ψ to include all leafgraphs. However, we will opt to use $\Psi(\mathcal{G})$ instead.

The next proposition demonstrates why the definition of the law of a graphing is consistent with that of the law of a finite graph.

Proposition 6.2. The law $\Psi(G)$ of a graph $G \in \mathbf{Graph}$ is the law of the measurable graphing $\mathcal{G} = (V(G), \{i_{xy} \ : \ xy \in E(G)\}, \mu)$ where μ is the uniform measure on $V(G)$, and $i_{xy} : V(G) \to V(G)$ maps x to y, y to x, and fixes the other vertices.

Proof. Since $\operatorname{Aut}(G)$ partitions the vertex set of G, $V(G) = \bigsqcup_{j=1}^{k} \operatorname{Aut}(G)j$. Furthermore, $|\operatorname{Aut}(G)j| \cdot \chi_A[G_j, j] = |\{x \in \operatorname{Aut}(G)j \ : \ [G_j, j] \in A\}|$, and $[G_x, x] = [G_j, j]$ because x and j are in the same orbit. Then

$$\begin{aligned}\Psi(G)(A) &= \sum_{j=1}^{k} \frac{|\operatorname{Aut}(G)j| \cdot \chi_A[G_j, j]}{|V(G)|} \\ &= \sum_{j=1}^{k} \frac{|\{x \in \operatorname{Aut}(G)j \ : \ [G_x, x] \in A\}|}{|V(G)|} \\ &= \frac{\left|\bigsqcup_{j=1}^{k}\{x \in \operatorname{Aut}(G)j \ : \ [G_x, x] \in A\}\right|}{|V(G)|} \\ &= \frac{|\{x \in V(G) \ : \ [G_x, x] \in A\}|}{|V(G)|}\end{aligned}$$

for all Borel subsets A of $\mathbf{Gr}$. In particular,

$$\Psi(G)(T_r(\mathbf{Gr}, \alpha)) = \mu(\{x \in V(G) \ : \ [B_{G_x}(x, r), x] = \alpha\})$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$. Hence $\Psi(G) = \Psi(\mathcal{G})$. □

To bridge the gap between the law of $\mathcal{G}$ and μ, the reader is encouraged to study the following proposition, which links the two measures.

Proposition 6.3. Let $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ be a measurable graphing. If $g : \mathbf{Gr} \to \mathbb{R}$ is a Borel function, then

$$\int_{\mathbf{Gr}} g \ d\Psi(\mathcal{G}) = \int_X g[\mathcal{L}_x, x] \ d\mu(x).$$

Proof. Define the function $q : (X, \mu) \to (\mathbf{Gr}, \Psi(\mathcal{G}))$ by $q(x) = [\mathcal{L}_x, x]$ for all $x \in X$. Observe that

$$q(y) \in T_r(\mathbf{Gr}, \alpha) \quad \Leftrightarrow \quad [\mathcal{L}_y, y] \in T_r(\mathbf{Gr}, \alpha) \quad \Leftrightarrow \quad [B_{\mathcal{L}_y}(y, r), y] = \alpha,$$

which means

$$q^{-1}(T_r(\mathbf{Gr}, \alpha)) = \{x \in X \ : \ [B_{\mathcal{L}_x}(x, r), x] = \alpha\}.$$

Furthermore, $B_{\mathcal{L}}(x, r) = B_{\mathcal{L}_x}(x, r)$. Then

$$\mu(q^{-1}(T_r(\mathbf{Gr}, \alpha))) = \mu(\{x \in X \ : \ [B_{\mathcal{L}_x}(x, r), x] = \alpha\}) = \Psi(\mathcal{G})(T_r(\mathbf{Gr}, \alpha))$$

for all $r \in \mathbb{N}$ and $\alpha \in U_r$, and so $q_*(\mu) = \Psi(\mathcal{G})$. Hence

$$\int_{\mathbf{Gr}} g \ d\Psi(\mathcal{G}) = \int_{\mathbf{Gr}} g \ dq_*(\mu) = \int_X (g \circ q) \ d\mu,$$

as required. □

Although the following result was shown before in this author's Honours project [Art11], the following argument presents another, more suitable, viewpoint.

Proposition 6.4. If $G \in \mathbf{Graph}$, then $\Psi(G)$ is unimodular.

Proof. Define the relation $S = \{(x, y) \in V(G) \times V(G) \ : \ xy \in E(G)\}$. Observe that S is symmetric; that is, $(x, y) \in S$ if and only if $(y, x) \in S$. Furthermore, $xy \in E(G)$ if and only if $y \in N_G(x)$, and $N_G(x) = N_{G_x}(x)$. Then

$$\begin{aligned}
\int \sum_{y \in N_H(x)} f[H, x, y] \ d\Psi(G)[H, x] &= \frac{1}{|V(G)|} \sum_{x \in V(G)} \sum_{y \in N_G(x)} f[G_x, x, y] \\
&= \frac{1}{|V(G)|} \sum_{(x,y) \in S} f[G_x, x, y] \\
&= \frac{1}{|V(G)|} \sum_{(y,x) \in S} f[G_x, x, y] \\
&= \frac{1}{|V(G)|} \sum_{(y,x) \in S} f[G_y, x, y] \\
&= \frac{1}{|V(G)|} \sum_{y \in V(G)} \sum_{x \in N_G(y)} f[G_y, x, y] \\
&= \int \sum_{x \in N_H(y)} f[H, x, y] \ d\Psi(G)[H, y]
\end{aligned}$$

where the fourth equality holds because $G_x = G_y$ whenever x is adjacent to y. □

Consider the measurable graphing $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ whose leafgraph is $\mathcal{L}$. Let $S_{\mathcal{L}} = \{(x, y) \in X \times X \ : \ xy \in E(\mathcal{L})\}$ and

$$\vec{\mu}(B) = \int_X |\{y \in N_{\mathcal{L}}(x) \ : \ (x, y) \in B\}| \ d\mu(x)$$

for all Borel subsets B of $S_{\mathcal{L}}$. For convenience, we will use ι to denote two different functions. The reader should already be familiar with the first of these functions from Definition 5.2. Let

$$\begin{aligned}
\iota : \vec{\mathbf{Gr}} &\to \vec{\mathbf{Gr}} \\
[G, x, y] &\mapsto [G, y, x]
\end{aligned}$$

and

$$\begin{aligned}
\iota : S_{\mathcal{L}} &\to S_{\mathcal{L}} \\
(x, y) &\mapsto (y, x),
\end{aligned}$$

which are both involutions. As for measures on $\mathbf{Gr}$, there is a similar notion of involution invariance for measures on X.

Definition 6.3. A measure μ on X is *involution invariant* if $\iota_*(\vec{\mu}) = \vec{\mu}$.

6.2 Laws of graphings are unimodular

With the basic tools in hand, we may now construct a proof that laws of graphings, when dealing with unimodularity, behave in the same way as laws of finite graphs.

For the remainder of this section, let $B_A = \{(x, y) \in S_{\mathcal{L}} \ : \ [\mathcal{L}_x, x, y] \in A\}$ and $A_B = \{[G, x, y] \in \vec{\mathbf{Gr}} \ : \ (x, y) \in B\}$ for all Borel subsets A of $\vec{\mathbf{Gr}}$ and B of $S_{\mathcal{L}}$.

Proposition 6.5. If A is a Borel subset of $\vec{\mathbf{Gr}}$, then $\chi_A[\mathcal{L}_x, x, y] = \chi_{B_A}(x, y)$ for all $(x, y) \in S_{\mathcal{L}}$. If B is a Borel subset of $S_{\mathcal{L}}$, then $\chi_B(x, y) = \chi_{A_B}[\mathcal{L}_x, x, y]$ for all $(x, y) \in S_{\mathcal{L}}$. Furthermore,

$$f_A[\mathcal{L}_x, x] := |\{y \in N_{\mathcal{L}}(x) \ : \ [\mathcal{L}_x, x, y] \in A\}| = \sum_{y \in N_{\mathcal{L}}(x)} \chi_A[\mathcal{L}_x, x, y]$$

and

$$|\{y \in N_{\mathcal{L}}(x) \ : \ (x, y) \in B\}| = \sum_{y \in N_{\mathcal{L}}(x)} \chi_B(x, y)$$

for all Borel subsets A of $\vec{\mathbf{Gr}}$ and B of $S_{\mathcal{L}}$.

Lemma 6.1. If B is a Borel subset of $S_{\mathcal{L}}$, then

$$\vec{\mu}(B) = \int_X \sum_{y \in N_{\mathcal{L}}(x)} \chi_B(x, y) \ d\mu(x).$$

Proof. By Proposition 6.5,

$$\int_X |\{y \in N_{\mathcal{L}}(x) \ : \ (x, y) \in B\}| \ d\mu(x) = \int_X \sum_{y \in N_{\mathcal{L}}(x)} \chi_B(x, y) \ d\mu(x),$$

and the result follows. □

Lemma 6.2. If A and B are Borel subsets of $\vec{\mathbf{Gr}}$ and $S_{\mathcal{L}}$, respectively, then $A_{\iota(B)} = \iota(A_B)$ and $B_{\iota(A)} = \iota(B_A)$.

Theorem 6.6. Let $\mathcal{G} = (X, i_1, i_2, \dots, i_k, \mu)$ be a measurable graphing. The law $\Psi(\mathcal{G})$ is involution invariant if and only if μ is involution invariant.

Proof. Suppose that $\Psi(\mathcal{G})$ is involution invariant. Let B be a Borel subset of $S_{\mathcal{L}}$. Proposition 6.5, Lemma 6.1, and Lemma 6.2 tell us that

$$\vec{\mu}(\iota(B)) = \int_{\mathbf{Gr}} \sum_{y \in N_{\mathcal{L}}(x)} \chi_{\iota(A_B)}[\mathcal{L}_x, x, y] \ d\Psi(\mathcal{G})[\mathcal{L}_x, x],$$

and we know that the right-hand side is equal to

$$\int_{\mathbf{Gr}} |\{y \in N_{\mathcal{L}}(x) \ : \ [\mathcal{L}_x, x, y] \in \iota(A_B)\}| \ d\Psi(\mathcal{G})[\mathcal{L}_x, x] = \vec{\Psi}(\mathcal{G})(\iota(A_B)),$$

which means $\iota_*(\vec{\mu})(B) = \vec{\Psi}(\mathcal{G})(\iota(A_B))$. A similar argument shows that $\vec{\mu}(B) = \vec{\Psi}(\mathcal{G})(A_B)$. Since $\Psi(\mathcal{G})$ is involution invariant, we see that $\iota_*(\vec{\mu}) = \vec{\mu}$.

Conversely, assume that μ is involution invariant. Let A be a Borel subset of $\vec{\mathbf{Gr}}$. By Proposition 6.3,

$$\vec{\Psi}(\mathcal{G})(\iota(A)) = \int_X f_{\iota(A)}[\mathcal{L}_x, x] \ d\mu(x),$$

and the right-hand side is equal to $\vec{\mu}(\iota(B_A))$ using Proposition 6.5, Lemma 6.1, and Lemma 6.2. That is, $\vec{\Psi}(\mathcal{G})(\iota(A)) = \vec{\mu}(\iota(B_A))$. Analogously, $\vec{\Psi}(\mathcal{G})(A) = \vec{\mu}(B_A)$. Then $\iota_*(\vec{\Psi}(\mathcal{G})) = \vec{\Psi}(\mathcal{G})$ because μ is involution invariant. □

The question that remains is whether a measure μ from some measurable graphing is *always* involution invariant. In fact, the answer to this question is affirmative. However, to prove this result, we consider a more general situation.

Definition 6.4. Let X be a Borel space; let E be a countable Borel equivalence relation on X. A *general graphing* is a tuple $\mathcal{G} = (X, \Gamma, \mu)$ where $\Gamma \subseteq E$ is an antireflexive and symmetric Borel relation.

Intimately related to this type of graphing is the concept of invariance under equivalence relations, defined below, which is discussed more thoroughly in a set of lecture notes by Alexander Kechris and Benjamin Miller [KM04].

Definition 6.5. Let X be a Borel space; let E be a countable Borel equivalence relation on X. A measure μ on X is *E-invariant* if for all Borel bijections $f : A \to B$ where A and B are Borel subsets of X and $\mathrm{gr}(f) \subseteq E$, we have $\mu(A) = \mu(B)$.

Using the notation of Kechris and Miller, define the measures M and M' as follows:

$$M(A) = \int_X |\{y \in X \ : \ (x, y) \in A\}| \ d\mu(x)$$

and

$$M'(A) = \int_X |\{y \in X \ : \ (y, x) \in A\}| \ d\mu(x)$$

for all Borel subsets A of E.

Proposition 6.7. If $M = M'$, then μ is E-invariant.

Proof. To show that μ is E-invariant, let $f : A \to B$ be a Borel bijection for some Borel subsets A and B of X. Note that $B = f(A)$ because f is a bijection. Suppose that $\mathrm{gr}(f) \subseteq E$ where $\mathrm{gr}(f)$ is Borel. Then

$$M(\mathrm{gr}(f)) = \int_A |\{y \in X \ : \ y = f(x)\}| \ d\mu(x) = \int_A |\{f(x)\}| \ d\mu(x) = \mu(A)$$

and

$$M'(\mathrm{gr}(f)) = \int_{f(A)} |\{y \in A \ : \ x = f(y)\}| \ d\mu(x) = \int_{f(A)} |\{f^{-1}(x)\}| \ d\mu(x) = \mu(f(A))$$

are equal because $M = M'$ by assumption. That is, $\mu(A) = \mu(f(A)) = \mu(B)$. ☐

Kechris and Miller prove that the converse is also true [KM04, p. 57], which leads to the following corollary.

Corollary 6.8. The measure μ is E-invariant if and only if $M = M'$.

Now if the reader recalls, our definition of measurable graphing provides us with an equivalence relation, and this is precisely what we need to use Corollary 6.8.

Theorem 6.9. Let (X, μ) be a measure space. If $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ is a measurable graphing, then μ is $\sim_{\mathcal{G}}$-invariant.

Proof. Let $\Gamma = \langle i_1, i_2, \ldots, i_k \rangle$ be the free group generated by the involutions. Denote by E the equivalence relation $\sim_{\mathcal{G}}$. The countable group Γ acts on X in a Borel fashion as follows: $\gamma \cdot x = \gamma(x)$ for all $x \in X$ and $\gamma \in \Gamma$. Note that $E = E_\Gamma^X$ where

$$(x, y) \in E_\Gamma^X \quad \Leftrightarrow \quad \exists \gamma \in \Gamma \ \ \gamma \cdot x = y$$

because any $\gamma \in \Gamma$ can be written as the composition of the generators $i_1, i_2, \ldots, i_k$.

Furthermore, μ is Γ-invariant: if A is a Borel subset of X and $\gamma \in \Gamma$, then

$$\mu(\gamma(A)) = \mu(\gamma \cdot A) = \mu(A)$$

because $(i_j)_*(\mu) = \mu$ and again γ is a composition of $i_1, i_2, \ldots, i_k$. Using a proposition from the lectures notes by Kechris and Miller [KM04, p. 57], we see that μ is E-invariant. ☐

Corollary 6.10. The law of a measurable graphing $\mathcal{G} = (X, i_1, i_2, \ldots, i_k, \mu)$ is unimodular.

Proof. Note that $M|_{S_\mathcal{L}} = \vec{\mu}$ and $M'|_{S_\mathcal{L}} = \iota_*(\vec{\mu})$, so $\iota_*(\vec{\mu}) = \vec{\mu}$. Theorem 6.6 implies that the law $\Psi(\mathcal{G})$ of the measurable graphing $\mathcal{G}$ is unimodular. ☐

7 Open problems

The purpose of this section is to acquaint the reader with several interesting questions that have yet to be resolved.

David Aldous and Russell Lyons [AL07] asked the following in 2007, and it remains, in this author's eyes, one of the most important questions listed here.

Open Question 7.1. Is every unimodular measure the weak limit of a sequence of laws of finite graphs?

A related but weaker question is obtained by removing the finiteness condition.

Open Question 7.2. Is every unimodular measure the weak limit of a sequence of laws of measurable graphings?

The questions that follow, if true, combine to establish an affirmative answer to Open Question 7.1.

Open Question 7.3. Is every unimodular measure the law of some measurable graphing?

Open Question 7.4. Is the law of a measurable graphing the weak limit of a sequence of laws of finite graphs?

We would also like to link the notion of unimodularity with that of sofic groups. Such groups were introduced by Mikhael Gromov and Benjamin Weiss. We refer the reader to a survey by Vladimir Pestov of the known and unknown results [Pes08].

Recall that a Cayley graph of a group Γ is the pair

$$\mathrm{Cay}(\Gamma, S) = (\Gamma, \{(x, sx) \in \Gamma \times \Gamma \ : \ s \in S\})$$

where S is a set of generators of Γ.

Definition 7.1. A finitely generated group Γ is *sofic* if it has a finite symmetric set of generators S such that for all positive real numbers ε and $r \in \mathbb{N}$, there is a finite directed graph $G = (V, E)$ edge-labeled by S, which has a finite subset of vertices $V_0 \subseteq V$ satisfying

1. $\forall v \in V_0$, $B_G(v, r)$ is edge-labeled isomorphic to $B_{\mathrm{Cay}(\Gamma,S)}(1_\Gamma, r)$, and
2. $|V_0| \geq (1 - \varepsilon)|V|$.

Open Question 7.5. Is a group sofic if and only if the Dirac measure on its Cayley graph is the weak limit of a sequence of laws of finite graphs?

If we deviate from the general setting of rooted graphs introduced in this article, we may also consider expander graphs as the objects of study, as well as automorphism groups of graphs.

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