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NUMERICAL CALCULATION OF SINGULARITIES FOR GINZBURG-LANDAU FUNCTIONALS

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Abstract. We give results of numerical calculations of asymptotic behavior of critical points of a Ginzburg-Landau functional. We use both continuous and discrete steepest descent in connection with Sobolev gradients in order to study configurations of singularities.

1. Location of Singularities

Suppose $\epsilon > 0$ and d is a positive integer. Consider the problem of determining critical points of the functional ϕ_ϵ:

$$\phi_\epsilon(u) = \int_\Omega (\|\nabla u\|^2/2 + (|u|^2-1)^2/(4\epsilon^2)),\ u \in H^{1,2}(\Omega, C),\ u(z) = z^d,\ z \in \partial\Omega, \tag{1.1}$$

where Ω is the unit closed disk in C, the complex numbers. For each such $\epsilon > 0$, denote by $u_{\epsilon,d}$ a minimizer of (1.1).

In [1] it is indicated that for various sequences $\{\epsilon_n\}_{n=1}^\infty$ of positive numbers converging to 0, precisely d singularities develop for $u_{\epsilon_n,d}$ as $n \to \infty$. The open problem is raised (Problem 12, page 139 of [1]) concerning possible orientation of such singularities. Our calculations suggest that for a given d there are (at least) two resulting families of singularity configurations. Each configuration is formed by vertices of a regular $d-$gon centered at the origin of C, with each corresponding member of one configuration being about .6 times as large as a member of the other. A family of which we speak is obtained by rotating a configuration through some angle α. That this results in another possible configuration follows from the fact (page 88 of [1]) that if

$$v_{\epsilon,d}(z) = e^{-id\alpha}u_{\epsilon,d}(e^{i\alpha}z), z \in \Omega,$$

then $\phi_\epsilon(v_{\epsilon,d}) = \phi_\epsilon(u_{\epsilon,d})$ and $v_{\epsilon,d}(z) = z^d, z \in \partial\Omega$.

That there should be singularity patterns formed by vertices of regular $d-$gons has certainly been anticipated although it seems that no proof has been put forward. What we offer here is some numerical support for this proposition. What surprised us in this work is the indication of *two* families for each positive integer d.

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We explain how these two families were encountered. Our calculations use steepest descent with numerical Sobolev gradients ([3], [2]). One family appears using discrete steepest descent and the other appears when continuous steepest descent is closely tracked numerically. We can offer no explanation for this phenomenon but simply report it. For a given d, the family of singularities obtained with discrete steepest descent is closer to the origin (by about a factor of .6) than the corresponding family for continuous steepest descent. In either case, the singularities are closer to the boundary of Ω for larger d. It is emphasized that more than the usual caveats concerning the deduction of analytical facts from numerical calculations certainly apply here. We are using a descent method to calculate critical points of a highly singular object (for small ϵ, a graph of $|u_{\epsilon,d}|^2$ would appear as a plate of height one above Ω with d slim tornadoes coming down to zero). Moreover for each d as indicated above, one expects a continuum of critical points (one obtained from another by rotation) from which to 'choose'. A feature of continuous steepest descent method with Sobolev gradients is that it tends to pick out the nearest (in perhaps some non-Euclidean sense) critical point to the starting estimate. Such methods are suited to problems in which there are many critical points. In addition, the topography of ϕ_ϵ over all competing functions seems rather severe with critical points having rather small support. This all makes for a fairly difficult calculation which calls for more computing power than is available to us at the moment. This is particularly true if one seeks evidence that as $d \to \infty$, then points of developing singularities approach $\partial\Omega$. In our opinion, owing to the importance of this problem, independent and more extensive calculations should be made.

Some questions. Are there more than two (even infinitely many) families of singularities for each d? Does some other descent method (or some other method entirely) lead one to new configurations? Are there in fact configurations which are not symmetric about the origin?

2. Description of Method

We indicate how to construct a Sobolev gradient for (1.1). We use an equivalent real formulation of (1.1) and regard ϕ_ϵ as a function from $H = H^{1,2}(\Omega, R)^2$ to R. For $u \in H$, $\phi'_\epsilon(u)$ is a continuous linear functional on H. Thus there is a unique member of H, called $(\nabla\phi_\epsilon)(u)$, such that

$$\phi'_\epsilon(u)h = \langle h, (\nabla\phi_\epsilon)(u)\rangle_H,\ u \in H,\ h \in H_0, \tag{2.1}$$

where H_0 is the subspace of H consisting of those members of H which are zero on $\partial\Omega$. The reader might refer to [3] or [2] for more details on an explicit construction of this gradient.

Once a gradient function for ϕ_ϵ is available there are two corresponding steepest descent processes, continuous steepest descent and discrete steepest descent.

Continuous steepest descent consists of picking $x \in H$ and determining $z : [0,\infty) \to H$ such that

$$z(0) = x,\ z'(t) = -(\nabla\phi_\epsilon)(z(t)),\ t \geq 0. \tag{2.2}$$

For each $\epsilon > 0$, critical points $u_{\epsilon,d} \in H$ are sought so that

$$u_{\epsilon,d} = \lim_{t\to\infty} z(t),$$

or at least so that

$$u_{\epsilon,d} = \lim_{n\to\infty} z(t_n)$$

for some unbounded increasing sequence $\{t_n\}_{n=1}^{\infty}$ of positive numbers.

For fixed $\epsilon > 0$ discrete steepest descent, on the other hand, consists of picking $x \in H$ and determining $\{z_n\}_{n=1}^{\infty}$ so that

$$z_{n+1} = z_n - \delta_n(\nabla\phi_\epsilon)(z_n),\ n = 1, 2, \ldots, \tag{2.3}$$

where δ_n is chosen to be the smallest positive local minimum δ of

$$\phi_\epsilon(z_n - \delta(\nabla\phi_\epsilon)(z_n)),\ \delta \geq 0.$$

Critical points $u_{\epsilon,d}$ of ϕ_ϵ are sought as a limit of a subsequence of $\{z_n\}_{n=1}^{\infty}$.

In the case of either continuous steepest descent or discrete steepest descent we are interested in asymptotic behavior of $u_{\epsilon,d}$ as $\epsilon \to 0$. For computations we seek a critical point of $\phi_{\epsilon,d}$ for 'small' ϵ as indicated in the following section. As explained in [1], there is not a limit in $H^{1,2}(\Omega)$ of $u_{\epsilon,d}$ as $\epsilon \to 0$ but that $u_{\epsilon,d}$ becomes more nearly singular as $\epsilon \to 0$.

For calculations we use a finite dimensional version of the above. The region Ω is broken into pieces using some number (180 to 400, depending on d) of evenly spaced radii together with 40 to 80 concentric circles. References [2],[3] contain details of Sobolev gradient construction in these finite dimensional settings. We mention that in our results, $u = \lim_{t\to\infty} z(t)$ appears to exist in the case of continuous steepest descent and $u = \lim_{n\to\infty} z_n$ appears to exist in the case of discrete steepest descent. Thus no 'taking of subsequences' seems to be necessary.

3. Results

For continuous steepest descent, using $d = 2, \ldots, 10$ we started each steepest descent iteration with a finite dimensional version of $u_{\epsilon,d}(z) = z^d$. To emulate continuous steepest descent, we used discrete steepest descent with small step size (on the order of .0001) instead of the optimal step size of (2.3). In all runs reported on here we used $\epsilon = 1/40$ except for the discrete steepest descent run with $d = 2$. In that case $\epsilon = 1/100$ was used (for $\epsilon = 1/40$ convergence seemed not to be forthcoming in the single precision code used - the value .063 given is likely smaller than a successful run with $\epsilon = 1/40$ would give). Runs with somewhat larger ϵ yielded a similar pattern except the corresponding singularities were a little farther from the origin. In all cases we found d singularities arranged on a regular d-gon centered at the origin.

Results for continuous steepest descent are indicated by the following pairs:

$$(2, .15), (3, .25), (4, .4), (5, .56), (6, .63), (7, .65), (8, .7), (9, .75), (10, .775)$$

where a pair (d, r) above indicates that a (near) singularity of $u_{\epsilon,d}$ was found at a distance r from the origin with $\epsilon = 1/40$. In each case the other $d - 1$ singularities are located by rotating the first one through an angle that is an integral multiple of $2\pi/d$.

Results for discrete steepest descent are indicated by the following pairs:

$$(2, .063), (3, .13), (4, .18), (5, .29), (6, .34), (7, .39), (8, .44), (9, .48), (10, .5)$$

using the same conventions as for continuous steepest descent. Computations with a finer mesh would surely yield more precise results.

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