### LARGE DATA AND ZERO NOISE LIMITS OF GRAPH-BASED SEMI-SUPERVISED LEARNING ALGORITHMS \* 2

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Abstract. Scalings in which the graph Laplacian approaches a differential operator in the 5 large graph limit are used to develop understanding of a number of algorithms for semi-supervised 6 learning; in particular the extension, to this graph setting, of the probit algorithm, level set and kriging methods, are studied. Both optimization and Bayesian approaches are considered, based 8 9 around a regularizing quadratic form found from an affine transformation of the Laplacian, raised to a, possibly fractional, exponent. Conditions on the parameters defining this quadratic form are 10 identified under which well-defined limiting continuum analogues of the optimization and Bayesian 11 semi-supervised learning problems may be found, thereby shedding light on the design of algorithms 12 in the large graph setting. The large graph limits of the optimization formulations are tackled 13 through  $\Gamma$ -convergence, using the recently introduced  $TL^p$  metric. The small labelling noise limit 14 of the Bayesian fomulations are also identified, and contrasted with pre-existing harmonic function 15 approaches to the problem. 16

Key words. Semi-supervised learning, Bayesian inference, higher-order fractional Laplacian, 17 asymptotic consistency, kriging. 18

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### 1. Introduction. 20

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**1.1.** Context. This paper is concerned with the semi-supervised learning prob-21 lem of determining labels on an entire set of (feature) vectors  $\{x_i\}_{i \in \mathbb{Z}}$ , given (possibly 22 noisy) labels  $\{y_j\}_{j\in Z'}$  on a subset of feature vectors with indices  $j\in Z'\subset Z$ . To be 23 concrete we will assume that the  $x_i$  are elements of  $\mathbb{R}^d$ ,  $d \ge 2$ , and consider the binary 24 classification problem in which the  $y_i$  are elements of  $\{\pm 1\}$ . Our goal is to characterize 25 algorithms for this problem in the large data limit where  $n = |Z| \rightarrow \infty$ ; additionally 26 we will study the limit where the noise in the label data disappears. Studying these 27 limits yields insight into the classification problem and algorithms for it. 28

Semi-supervised learning as a subject has been developed primarily over the last 29 two decades and the references [51, 52] provide an excellent source for the historical 30 context. Graph based methods proceed by forming a graph with n nodes Z, and use 31 the unlabelled data  $\{x_j\}_{j\in \mathbb{Z}}$  to provide an  $n \times n$  weight matrix W quantifying the 32 affinity of the nodes of the graph with one another. The labelling information on Z'33 is then spread to the whole of Z, exploiting these affinities. In the absence of labelling 34 information we obtain the problem of unsupervised learning; for example the spectrum 35 of the graph Laplacian L forms the basis of widely used spectral clustering methods 36 [3, 34, 45]. Other approaches are combinatorial, and largely focussed on graph cut 37 methods [8, 9, 36]. However relaxation and approximation are required to beat the 38 combinatorial hardness of these problems [31] leading to a range of methods based 39 on Markov random fields [30] and total variation relaxation [40]. In [52] a number 40

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of new approaches were introduced, including label propagation and the generaliza-41 tion of kriging, or Gaussian process regression [47], to the graph setting [53]. These 42 regression methods opened up new approaches to the problem, but were limited in 43 scope because the underlying real-valued Gaussian process was linked directly to the 44 categorical label data which is (arguably) not natural from a modelling perspective; 45 see [33] for a discussion of the distinctions between regression and classification. The 46 logit and probit methods of classification [48] side-step this problem by postulating a 47 link function which relates the underlying Gaussian process to the categorical data, 48 amounting to a model linking the unlabelled and labelled data. The support vector 49 machine [7] makes a similar link, but it lacks a natural probabilistic interpretation. 50

The probabilistic formulation is important when it is desirable to equip the clas-51 sification with measures of uncertainty. Hence, we will concentrate on the probit 52 algorithm in this paper, and variants on it, as it has a probabilistic formulation. 53 The statement of the probit algorithm in the context of graph based semi-supervised 54 learning may be found in [6]. An approach bridging the combinatorial and Gaussian 55 process approaches is the use of Ginzburg-Landau models which work with real num-56 bers but use a penalty to constrain to values close to the range of the label data  $\{\pm 1\}$ ; 57 these methods were introduced in [4], large data limits studied in [15, 42, 44], and 58 given a probabilistic interpretation in [6]. Finally we mention the Bayesian level set 59 method. This approach takes the idea of using level sets for inversion in the class of 60 interface problems [11] and gives it a probabilistic formulation which has both theo-61 retical foundations and leads to efficient algorithms [28]; classification may be viewed 62 as an interface problem on a graph (a graph cut is an interface for example) and thus 63 the Bayesian level set method is naturally extended to this setting as shown in [6]. 64 As part of this paper we will show that the probit and Bayesian level set methods are 65 closely related. 66

A significant challenge for the field, both in terms of algorithmic development, 67 and in terms of fundamental theoretical understanding, is the setting in which the 68 volume of unlabelled data is high, relative to the volume of labelled data. One way 69 to understand this setting is through the study of large data limits in which  $n = |Z| \rightarrow$ 70  $\infty$ . This limit is studied in [46], and was addressed more recently under different 71 assumptions in [21]. Both papers assume that the unlabelled data is drawn i.i.d. 72 from a measure with Lebesgue density on a subset of  $\mathbb{R}^d$ , but the assumptions on 73 graph construction differ: in [46] the graph bandwidth is fixed as  $n \to \infty$  resulting 74 in the limit of the graph Laplacian being a non-local operator, whilst in [21] the 75 bandwidth vanishes in the limit resulting in the limit being a weighted Laplacian 76 (divergence form elliptic operator). 77

In [32] it is demonstrated that algorithms based on use of the discrete Dirichlet 78 energy computed from the graph Laplacian can behave poorly for  $d \ge 2$ , in the large 79 data limit, if they attempt pointwise labelling. In [50] it is argued that use of quadratic 80 forms based on powers  $\alpha > \frac{d}{2}$  of the graph Laplacian can ameliorate this problem. 81 Our work, which studies a range of algorithms all based on optimization or Bayesian 82 formulations exploiting quadratic forms, will take this body of work considerably 83 further, proving large data limit theorems for a variety of algorithms, and showing 84 the role of the parameter  $\alpha$  in this infinite data limit. In doing so we shed light 85 on the difficult question of how to scale and tune algorithms for graph based semi-86 supervised learning; in particular we state limit theorems of various kinds which 87 require, respectively, either  $\alpha > \frac{d}{2}$  or  $\alpha > d$  to hold. We also study the small noise 88 limit and show how both the probit and Bayesian level set algorithms coincide and, 89 furthermore, provide a natural generalization of the harmonic functions approach of 90

<sup>91</sup> [53, 54], one which is arguably more natural from a modeling perspective.

Our large data limit theorems concern the maximum a posteriori (MAP) estimator rather than a Bayesian posterior distribution. However two remarkable recent papers [20, 19] demonstrate a methodology for proving limit theorems concerning Bayesian posterior distributions themselves, exploiting the variational characterization of Bayes theorem; extending the work in those papers to the algorithms considered in this paper would be of great interest.

**1.2.** Our Contribution. We derive a canonical continuum inverse problem 98 which characterizes graph based semi-supervised learning: find function  $u: \Omega \subset \mathbb{R}^d \mapsto$ 99  $\mathbb{R}$  from knowledge of sign(u) on  $\Omega' \subset \Omega$ . <sup>1</sup> The latent variable u characterizes the 100 unlabelled data and its sign is the labelling information. This highly ill-posed inverse 101 problem is potentially solvable because of the very strong prior information provided 102 by the unlabelled data; we characterize this information via a mean zero Gaussian 103 process prior on u with covariance operator  $\mathcal{C} \propto (\mathcal{L} + \tau^2 I)^{-\alpha}$ . The operator  $\mathcal{L}$  is a 104 weighted Laplacian found as a limit of the graph Laplacian, and as a consequence 105 depends on the distribution of the unlabelled data. 106

In order to derive this canonical inverse problem we study the probit and Bayesian 107 level set algorithms for semi-supervised learning. We build on the large unlabelled 108 data limit setting of [21]. In this setting there is an intrinsic scaling parameter  $\varepsilon_n$  that 109 characterizes the length scale on which edge weights between nodes are significant; 110 the analysis identifies a lower bound on  $\varepsilon_n$  which is necessary in order for the graph 111 to remain connected in the large data limit and under which the graph Laplacian 112 L converges to a differential operator  $\mathcal{L}$  of weighted Laplacian form. The work uses 113  $\Gamma$ -convergence in the  $TL^2$  optimal transport metric, introduced in [21], and proves 114 convergence of the quadratic form defined by L to one defined by  $\mathcal{L}$ . We make the 115 following contributions which significantly extend this work to the semi-supervised 116 learning setting. 117

- We prove  $\Gamma$ -convergence in  $TL^2$  of the quadratic form defined by  $(L + \tau^2 I)^{\alpha}$ to that defined by  $(\mathcal{L} + \tau^2 I)^{\alpha}$  and identify parameter choices in which the limiting Gaussian measure with covariance  $(\mathcal{L} + \tau^2 I)^{-\alpha}$  is well-defined. See Theorems 1, 4 and Proposition 5.
- We introduce large data limits of the probit and Bayesian level set problem formulations in which the volume of unlabelled data  $n = |Z| \rightarrow \infty$ , distinguishing between the cases where the volume of labelled data |Z'| is fixed and where |Z'|/n is fixed. See section 4 for the function space analogues of the of the graph based algorithms introduced in 3.
- We use the theory of  $\Gamma$ -convergence to derive a continuum limit of the probit algorithm when employed in MAP estimation mode; this theory demonstrates the need for  $\alpha > \frac{d}{2}$  and an upper bound on  $\varepsilon_n$  in the large data limit where the volume of labelled data |Z'| is fixed. See Theorems 10 and 11
- We use the properties of Gaussian measures on function spaces to write down well defined limits of the probit and Bayesian level set algorithms, when employed in Bayesian probabilistic mode, to determine the posterior distribution on labels given observed data; this theory demonstrates the need for  $\alpha > \frac{d}{2}$  in order for the limiting probability distribution to be meaningful for both large data limits; indeed, depending on the geometry of the domain from which the feature vectors are drawn, it may require  $\alpha > d$  for the case where the volume

<sup>1</sup> We note that throughout the paper  $\Omega$  is the physical domain, and not the set of events of a probability space.

of labelled data is fixed. See Theorem 4 and Proposition 5 for these conditions on  $\alpha$ , and for details of the limiting probability measures see equations (21), (22), (23) and (24).

• We show that the probit and Bayesian level set method have a common Bayesian inverse problem limit, mentioned above, by studying their weak limits as noise levels on the label data tends to zero. See Theorems 8 and 14.

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• We provide careful numerical experiments which illusrate the large graph limits introduced and studied in this paper; see section 5.

**1.3.** Paper Structure. In section 2 we study a family of quadratic forms which 146 arise naturally in all the algorithms that we study. By means of the  $\Gamma$ -convergence 147 techniques pioneered in [21] we show that these quadratic forms have a limit defined 148 by families of differential operators in which the finite graph parameters appear in an 149 explicit and easily understood fashion. Section 3 is devoted to the definition of the 150 three graph based algorithms that we study in this paper: the probit and Bayesian 151 level set algorithms, and the graph analogue of kriging. In section 4 we write down the 152 function space limits of these algorithms, obtained when the volume n of unlabelled 153 data tends to infinity, and in the case of the maximum a posteriori estimator for 154 probit use  $\Gamma$ -convergence to study large graph limits rigorously; we also show that 155 the probit and Bayesian level set algorithms have a common zero noise limit. Section 5 156 contains numerical experiments for the function space limits of the algorithms, in both 157 optimization (MAP) and sampling (fully Bayesian MCMC) modalities. We conclude 158 in section 6 with a summary and directions for future research. All proofs are given 159 in the Appendix, section 7. This choice is made in order to separate the form and 160 implications of the theory from the proofs; both the statements and proofs comprise 161 the contributions of this work, but since they may be of interest to different readers 162 they are separated, by use of the Appendix. 163

## <sup>164</sup> 2. Key Quadratic Form and Its Limits.

**2.1. Graph Setting.** From the unlabelled data  $\{x_j\}_{j=1}^n$  we construct a weighted graph G = (Z, W) where  $Z = \{1, \dots, n\}$  are the vertices of the graph and W the edge weight matrix; W is assumed to have entries  $\{w_{ij}\}$  between nodes i and j given by

$$w_{ij} = \eta_{\varepsilon}(|x_i - x_j|).$$

We will discuss choice of the function  $\eta_{\varepsilon} : \mathbb{R} \to \mathbb{R}^+$  in detail below; heuristically it should be thought of as proportional to a mollified Dirac mass, or a characteristic function of a small interval. From W we construct the graph Laplacian as follows. We define the diagonal matrix  $D = \text{diag}\{d_{ii}\}$  with entries  $d_{ii} = \sum_{j \in \mathbb{Z}} w_{ij}$ . We can then define the unnormalized graph Laplacian L = D - W. Our results may be generalized to the normalized graph Laplacian  $L = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$  and we will comment on this in the conclusions.

**2.2. Quadratic Form.** We view  $u : Z \mapsto \mathbb{R}$  as a vector in  $\mathbb{R}^n$  and define the quadratic form

$$\langle u, Lu \rangle = \frac{1}{2} \sum_{i,j \in \mathbb{Z}} w_{ij} |u(i) - u(j)|^2;$$

here  $\langle \cdot, \cdot \rangle$  denotes the standard Euclidean inner-product on  $\mathbb{R}^n$ . This is the discrete Dirichlet energy defined via the graph Laplacian L and appears as a basic quantity in many unsupervised and semi-supervised learning algorithms. In this paper our <sup>180</sup> interest focusses on forms based on powers of L:

$$J_n^{(\alpha,\tau)}(u) = \frac{1}{2n} \langle u, A^{(n)} u \rangle$$

181 where

(1) 
$$A^{(n)} = (s_n L + \tau^2 I)^{\alpha}.$$

The sequence parameters  $s_n$  will be chosen appropriately to ensure that the quadratic form  $J_n^{(\alpha,\tau)}(u)$  converges to a well-defined limit as  $n \to \infty$ .

In addition to working in a set-up which results in a well-defined limit, we will also ask that this limit results in a quadratic form defined by a differential operator. This, of course, requires some form of localization and we will encode this as follows: we will assume that  $\eta_{\varepsilon}(\cdot) = \varepsilon^{-d} \eta(\cdot/\varepsilon)$ , inducing a Dirac mass approximation as  $\varepsilon \to 0$ ; later we will discuss how to relate  $\varepsilon$  to n. For now we state the assumptions on  $\eta$  that we employ throughout the paper:

<sup>190</sup> **Assumptions** 1 (on  $\eta$ ). The edge weight profile function  $\eta$  satisfies: <sup>191</sup> (K1)  $\eta(0) > 0$  and  $\eta(\cdot)$  continuous at the origin;

<sup>192</sup> (K2)  $\eta$  non-increasing;

$$(K3) \quad \int_0^\infty \eta(r) r^{d+1} dr < \infty$$

<sup>194</sup> Notice that assumption (K3) implies that

(2) 
$$\sigma_{\eta} \coloneqq \frac{1}{d} \int_{\mathbb{R}^d} \eta(h) |h|^2 dh < \infty \quad \text{and} \quad \beta_{\eta} \coloneqq \int_{\mathbb{R}^d} \eta(h) dh < \infty$$

<sup>195</sup> A notable fact about the limits that we study in the remainder of the paper is that <sup>196</sup> they depend on  $\eta$  only through the constants  $\sigma_{\eta}, \beta_{\eta}$ , provided Assumptions 1 hold <sup>197</sup> and  $\varepsilon = \varepsilon_n$  and  $s_n$  are chosen as appropriate functions of n.

## <sup>198</sup> 2.3. Limiting Quadratic Form.

<sup>199</sup> The limiting quadratic form is defined on an open and bounded set  $\Omega \subset \mathbb{R}^d$ .

**Assumptions** 2 (on  $\Omega$ ). We assume that  $\Omega$  is a connected, open and bounded subset of  $\mathbb{R}^d$ . We also assume that  $\Omega$  has  $C^{1,1}$  boundary.<sup>2</sup>

**Assumptions** 3 (on density  $\rho$ ). We assume that n feature vectors  $x_j \in \Omega$  are sampled i.i.d. from a probability measure  $\mu$  supported on  $\Omega$  with smooth Lebesgue density  $\rho$  bounded above and below by finite strictly positive constants  $\rho^{\pm}$  uniformly on  $\overline{\Omega}$ .

We index the data by  $Z = \{1, \dots, n\}$  and let  $\Omega_n = \{x_i\}_{i \in \mathbb{Z}}$  be the data set. This data set induces the empirical measure

$$\mu_n = \frac{1}{n} \sum_{i \in Z} \delta_{x_i}.$$

<sup>&</sup>lt;sup>2</sup>The assumption that  $\Omega$  is connected is not essential but makes stating the results simpler. We remark that a number of the results, and in particular the convergence of Theorem 1, hold if we only assume that the boundary of  $\Omega$  is Lipschitz. We need the stronger assumption in order to be able to employ elliptic regularity to characterize functions in fractional Sobolev spaces, see Section 2.4 and Lemma 16; this is essential to be able to define Gaussian measures on function spaces, and therefore needed to define a Bayesian approach in which uncertainty of classifiers may be estimated.

Given a measure  $\nu$  on  $\Omega$  we define the weighted Hilbert space  $L^2_{\nu} = L^2_{\nu}(\Omega; \mathbb{R})$  with inner-product

(3) 
$$\langle a,b\rangle_{\nu} = \int_{\Omega} a(x)b(x)\nu(dx)$$

and induced norm defined by the identity  $\|\cdot\|_{L^2_{\nu}}^2 = \langle\cdot,\cdot\rangle_{\nu}$ . Note that with these definitions we have

$$J_n^{(\alpha,\tau)}: L^2_{\mu_n} \mapsto [0,+\infty), \qquad J_n^{(\alpha,\tau)}(u) = \frac{1}{2} \langle u, A^{(n)} u \rangle_{\mu_n}$$

In what follows we apply a form of  $\Gamma$ -convergence to establish that for large *n* the quadratic form  $J_n^{(\alpha,\tau)}$  is well approximated by the limiting quadratic form

$$J_{\infty}^{(\alpha,\tau)}: L^{2}_{\mu} \mapsto [0,+\infty) \cup \{+\infty\}, \qquad J_{\infty}^{(\alpha,\tau)}(u) = \frac{1}{2} \langle u, \mathcal{A}u \rangle_{\mu}$$

Here  $\mu$  is the measure on  $\Omega$  with density  $\rho$ , and we define the  $L^2_{\mu}$  self-adjoint differential operator  $\mathcal{L}$  by

(4) 
$$\mathcal{L}u = -\frac{1}{\rho} \nabla \cdot (\rho^2 \nabla u), \quad x \in \Omega, \qquad \frac{\partial u}{\partial n} = 0, \quad x \in \partial \Omega$$

The operator  $\mathcal{A}$  is then defined by  $\mathcal{A} = (\mathcal{L} + \tau^2 I)^{\alpha}$ .

<sup>217</sup> We may now relate the quadratic forms defined by  $A^{(n)}$  and  $\mathcal{A}$ . The  $TL^2$  topology <sup>218</sup> is introduced in [21] and defined in the Appendix section 7.2.2 for convenience. The <sup>219</sup> following theorem is proved in section 7.4.

THEOREM 1. Let Assumptions 1-3 hold. Let  $\{\varepsilon_n\}_{n=1,2,...}$  be a positive sequence converging to zero, and such that

(5) 
$$\lim_{n \to \infty} \left(\frac{\log n}{n}\right)^{1/d} \frac{1}{\varepsilon_n} = 0 \qquad \text{if } d \ge 3,$$
$$\lim_{n \to \infty} \left(\frac{\log n}{n}\right)^{1/2} \frac{(\log n)^{\frac{1}{4}}}{\varepsilon_n} = 0 \qquad \text{if } d = 2,$$

<sup>222</sup> and assume that the scale factor  $s_n$  is defined by

(6) 
$$s_n = \frac{2}{\sigma_\eta n \varepsilon_n^2}$$

<sup>223</sup> Then, with probability one, we have

1. 
$$\Gamma - \lim_{n \to \infty} J_n^{(\alpha, \tau)} = J_{\infty}^{(\alpha, \tau)}$$
 with respect to the  $TL^2$  topology;

225 2. if 
$$\tau = 0$$
, any sequence  $\{u_n\}$  with  $u_n : \Omega_n \to \mathbb{R}$  satisfying  $\sup_n ||u_n||_{L^2_{\mu_n}} < \infty$   
226 and  $\sup_{n \in \mathbb{N}} J_n^{(\alpha,0)}(u_n) < \infty$  is pre-compact in the  $TL^2$  topology;

227 3. if 
$$\tau > 0$$
, any sequence  $\{u_n\}$  with  $u_n : \Omega_n \to \mathbb{R}$  satisfying  $\sup_{n \in \mathbb{N}} J_n^{(\alpha, \tau)}(u_n) < \infty$   
228 is pre-compact in the  $TL^2$  topology.

Remark 2. As we discuss in section 7.2.1 of the appendix,  $\Gamma$ -convergence and pre-229 compactness allow one to show that minimizers of a sequence of functionals converge 230 to the minimizer of the limiting functional. The results of Theorem 1 provide the 231  $\Gamma$ -convergence and pre-compactness of fractional Dirichlet energies, which are the key 232 term of the functionals, such as (10) below, that define the learning algorithms that we 233 study. In particular Theorem 1 enables us to prove the convergence, in the large data 234 limit  $n \to \infty$ , of minimizers of functionals such as (10) (i.e. of outcomes of learning 235 algorithms), as shown in Theorem 10. 236

237 **2.4. Function Spaces.** The operator  $\mathcal{L}$  given by (4) is uniformly elliptic as a 238 consequence of the assumptions on  $\rho$ , and is self-adjoint with respect to the inner 239 product (3) on  $L^2_{\mu}$ . By standard theory, it has a discrete spectrum:  $0 = \lambda_1 < \lambda_2 \leq \cdots$ , 240 where the fact that  $0 < \lambda_2$  uses the connectedness of the domain and the uniform 241 positivity of  $\rho$  on the domain. Let  $\varphi_i$  for  $i = 1, \ldots$  be the associated  $L^2_{\mu}$ -orthonormal 242 eigenfunctions. They form a basis of  $L^2_{\mu}$ .

By Weyl's law the eigenvalues of  $\{\lambda_j\}_{j\geq 1}$  of  $\mathcal{L}$  satisfy  $\lambda_j \approx j^{2/d}$ . For completeness a simple proof is proved in Lemma 27; the analogous and more general results applicable to the Laplace-Beltrami operator may be found in, Hörmander [27].

246 Spectrally defined Sobolev spaces. For  $s \ge 0$  we define

$$\mathcal{H}^{s}(\Omega) = \left\{ u \in L^{2}_{\mu} : \sum_{k=1}^{\infty} \lambda^{s}_{k} a^{2}_{k} < \infty \right\}$$

where  $a_k = \langle u, \varphi_k \rangle_{\mu}$  and thus  $u = \sum_k a_k \varphi_k$  in  $L^2_{\mu}$ . We note that  $\mathcal{H}^s(\Omega)$  is a Hilbert space with respect to the inner product

$$\langle\!\langle u, v \rangle\!\rangle_{s,\mu} = a_1 b_1 + \sum_{k=1}^{\infty} \lambda_k^s a_k b_k$$

where  $b_k = \langle v, \varphi_k \rangle_{\mu}$ . It follows from the definition that for any  $s \ge 0$ ,  $\mathcal{H}^s(\Omega)$  is isomorphic to a weighted  $\ell^2(\mathbb{N})$  space, where the weights are formed by the sequence  $1, \lambda_2^s, \lambda_3^s, \ldots$ 

In Lemma 16 in the Appendix section 7.1 we show that for any integer s > 0,  $\mathcal{H}^{s}(\Omega) \subset H^{s}(\Omega)$  where  $H^{s}(\Omega)$  is the standard fractional Sobolev space. More precisely we characterize  $\mathcal{H}^{s}(\Omega)$  as the set of those functions in  $H^{s}(\Omega)$  which satisfy the appropriate boundary condition and show that the norms of  $\mathcal{H}^{s}(\Omega)$  and  $H^{s}(\Omega)$ are equivalent on  $\mathcal{H}^{s}(\Omega)$ .

We also note that for any integer s and  $\theta \in (0, 1)$  the space  $\mathcal{H}^{s+\theta}$  is a interpolation space between  $\mathcal{H}^s$  and  $\mathcal{H}^{s+1}$ . In particular  $\mathcal{H}^{s+\theta} = [\mathcal{H}^s, \mathcal{H}^{s+1}]_{\theta,2}$ , where the real interpolation space used is as in Definition 3.3 of Abels [1]. This identification of  $\mathcal{H}^s$  follows from the characterization of interpolation spaces of weighted  $L^p$  spaces by Peetre [35], as referenced by Gilbert [24]. Together these facts allow us to characterize the Hölder regularity of functions in  $\mathcal{H}^s(\Omega)$ .

LEMMA 3. Under Assumptions 2-3, for all  $s \ge 0$  there exists a bounded, linear, extension mapping  $E : \mathcal{H}^{s}(\Omega) \to H^{s}(\mathbb{R}^{d})$ . That is for all  $f \in \mathcal{H}^{s}(\Omega), E(f)|_{\Omega} = f$  a.e. Furthermore:

(i) if  $s < \frac{d}{2}$  then  $\mathcal{H}^{s}(\Omega)$  embeds continuously in  $L^{q}(\Omega)$  for any  $q \le \frac{2d}{d-2s}$ ; (ii) if  $s > \frac{d}{2}$  then  $\mathcal{H}^{s}(\Omega)$  embeds continuously in  $C^{0,\gamma}(\Omega)$  for any  $\gamma < \min\{1, s - \frac{d}{2}\}$ .

<sup>268</sup> The proof is presented in the Appendix 7.1.

We note that this implies that when  $\alpha > \frac{d}{2}$  pointwise evaluation is well-defined in the limiting quadratic form  $J_{\infty}^{(\alpha,\tau)}$ ; this will be used in what follows to show that the the limiting labelling model obtained when |Z'| is fixed is well-posed.

272 **2.5.** Gaussian Measures of Function Spaces. Using the ellipticity of  $\mathcal{L}$ , 273 Weyl's law, and Lemma 3 allows us to characterize the regularity of samples of Gaus-274 sian measures on  $L^2_{\mu}$ . The proof of the following theorem is a straightforward ap-275 plication of the techniques in [17, Theorem 2.10] to obtain the Gaussian measures 276 on  $\mathcal{H}^s(\Omega)$ . Concentration of the measure on  $H^s$  and on  $C^{0,\gamma}(\Omega)$  then follows from Lemma 3. When  $\tau = 0$  we work on the space orthogonal to constants in order that C(defined in the theorem below) is well defined.

THEOREM 4. Let Assumptions 2-3 hold. Let  $\mathcal{L}$  be the operator defined in (4), and define  $\mathcal{C} = (\mathcal{L} + \tau^2 I)^{-\alpha}$ . For any fixed  $\alpha > \frac{d}{2}$  and  $\tau \ge 0$ , the Gaussian measure  $N(0, \mathcal{C})$  is well-defined on  $L^2_{\mu}$ . Draws from this measure are almost surely in  $H^s(\Omega)$ for any  $s < \alpha - \frac{d}{2}$ , and consequently in  $C^{0,\gamma}(\Omega)$  for any  $\gamma < \min\{1, \alpha - d\}$  if  $\alpha > d$ .

We note that if the operator  $\mathcal{L}$  has eigenvectors which are as regular as those of the Laplacian on a flat torus then the conclusions of Theorem 4 can be strengthened. Namely if in addition to what we know about  $\mathcal{L}$ , there is C > 0 such that

(7) 
$$\sup_{j\geq 1} \left( \|\varphi_j\|_{L^{\infty}} + \frac{1}{j^{1/d}} \operatorname{Lip}(\varphi_j) \right) \leq C$$

then the Kolmogorov continuity technique [17, Section 7.2.5] can be used to show additional Hölder continuity.

PROPOSITION 5. Let Assumptions 2–3 hold. Assume the operator  $\mathcal{L}$  satisfies condition (7) and define  $\mathcal{C} = (\mathcal{L} + \tau^2 I)^{-\alpha}$ . For any fixed  $\alpha > d/2$  and  $\tau \ge 0$ , the Gaussian measure  $N(0, \mathcal{C})$  is well-defined on  $L^2_{\mu}$ . Draws from this measure are almost surely in  $H^s(\Omega; \mathbb{R})$  for any  $s < \alpha - d/2$ , and in  $C^{0,\gamma}(\Omega; \mathbb{R})$  for any  $\gamma < \min\{1, \alpha - \frac{d}{2}\}$  if  $\alpha > \frac{d}{2}$ .

We note that in general one cannot expect that the operator  $\mathcal{L}$  satisfies the bound 292 (7). For example, for the ball there is a sequence of eigenfunctions which satisfy 293  $\|\varphi_k\|_{L^{\infty}} \sim \lambda_k^{(d-1)/4} \sim k^{(d-2)/(2d)}$ , see [25]. In fact this is the largest growth of eigen-294 functions possible, as on general domains with smooth boundary  $\|\varphi_k\|_{L^{\infty}} \lesssim \lambda_k^{(d-1)/4}$ 295 as follows from the work of Grieser, [25]. Analogous bounds have first been estab-296 lished for operators on manifolds without boundary by Hörmander, [27]. This bound 297 is rarely saturated as shown by Sogge and Zeldtich [39], but determining the scaling 298 for most sets and manifolds remains open. Establishing the conditions on  $\Omega$  under 299 which the Theorem 4 can be strengthened as in Proposition 5 is of great interest. 300

301 **3. Graph Based Formulations.** We now assume that we have access to label 302 data defined as follows. Let  $\Omega' \subset \Omega$  and let  $\Omega^{\pm}$  be two subsets of  $\Omega'$  such that

$$\Omega^+ \cup \Omega^- = \Omega', \quad \overline{\Omega^+} \cap \overline{\Omega^-} = \emptyset$$

<sup>303</sup> We will consider two labelling scenarios:

• Labelling Model 1.  $|Z'|/n \to \mathfrak{r} \in (0, \infty)$ . We assume that  $\Omega^{\pm}$  have positive Lebesgue measure. We assume that the  $\{x_j\}_{j\in\mathbb{N}}$  are drawn i.i.d. from measure  $\mu$ . Then if  $x_j \in \Omega^+$  we set  $y_j = 1$  and if  $x_j \in \Omega^-$  then  $y_j = -1$ . The label variables  $y_j$  are not defined if  $x_j \in \Omega \setminus \Omega'$  where  $\Omega' = \Omega^+ \cup \Omega^-$ . We assume dist $(\Omega^+, \Omega^-) > 0$  and define  $Z' \subset Z$  to be the subset of indices for which we have labels.

Labelling Model 2. |Z'| fixed as  $n \to \infty$ . We assume that  $\Omega^{\pm}$  comprise a fixed number of points,  $n^{\pm}$  respectively. We assume that the  $\{x_j\}_{j>n^++n^-}$  are drawn i.i.d. from measure  $\mu$  whilst  $\{x_j\}_{1\leq j\leq n^+}$  are a fixed set of points in  $\Omega^+$  and  $\{x_j\}_{n^++1\leq j\leq n^++n^-}$  are a fixed set of points in  $\Omega^-$ . We label these fixed points by  $y: \Omega^{\pm} \mapsto \{\pm 1\}$  as in Labelling Model 1. We define  $Z' \subset Z$  to be the subset of indices  $\{1, \dots, n^+ + n^-\}$  for which we have labels and  $\Omega' = \Omega^+ \cup \Omega^-$ . In both cases  $j \in Z'$  if and only if  $x_j \in \Omega'$ . But in Model 1 the  $x_j$  are drawn i.i.d. and

assigned labels when they lie in  $\Omega'$ , assumed to have positive Lebesgue measure; in

Model 2 the  $\{(x_j, y_j)\}_{j \in Z'}$  are provided, in a possibly non-random way, independently of the unlabelled data.

We will identify  $u \in \mathbb{R}^n$  and  $u \in L^2_{\mu_n}(\Omega; \mathbb{R})$  by  $u_j = u(x_j)$  for each  $j \in Z$ . Similarly, we will identify  $y \in \mathbb{R}^{n^+ + n^-}$  and  $y \in L^2_{\mu_n}(\Omega'; \mathbb{R})$  by  $y_j = y(x_j)$  for each  $j \in Z'$ . We may therefore write, for example,

$$\frac{1}{n}\langle u,Lu\rangle_{\mathbb{R}^n}=\langle u,Lu\rangle_{\mu_n}$$

where u is viewed as a vector on the left-hand side and a function on Z on the right-hand side.

The algorithms that we study in this paper have interpretations through both optimization and probability. The labels are found from a real-valued function  $u : Z \mapsto \mathbb{R}$  by setting  $y = S \circ u : Z \mapsto \mathbb{R}$  with S the sign function defined by

$$S(0) = 0;$$
  $S(u) = 1, u > 0;$  and  $S(u) = -1, u < 0.$ 

The objective function of interest takes the form

$$\mathsf{J}^{(n)}(u) = \frac{1}{2} \langle u, A^{(n)}u \rangle_{\mu_n} + r_n \Phi^{(n)}(u).$$

The quadratic form depends only on the unlabelled data, while the function  $\Phi^{(n)}$  is determined by the labelled data. Choosing  $r_n = \frac{1}{n}$  in Labeling Model 1 and  $r_n = 1$ in Labeling Model 2 ensures that the total labelling information remains of  $\mathcal{O}(1)$  in the large *n* limit. Probability distributions constructed by exponentiating multiples of  $J^{(n)}(u)$  will be of interest to us; the probability is then high where the objective function is small, and vice-versa. Such probabilities represent the Bayesian posterior distribution on the conditional random variable u|y.

**332 3.1. Probit.** The probit algorithm on a graph is defined in [6] and here generalized to a quadratic form based on  $A^{(n)}$  rather than L. We define

(8) 
$$\Psi(v;\gamma) = \frac{1}{\sqrt{2\pi\gamma^2}} \int_{-\infty}^{v} \exp\left(-t^2/2\gamma^2\right) \mathrm{d}t$$

334 and then

(9) 
$$\Phi_{\mathbf{p}}^{(n)}(u;\gamma) = -\sum_{j \in Z'} \log \Big( \Psi(y_j u_j;\gamma) \Big).$$

The function  $\Psi$  and its logarithm are shown in Figure 1 in the case  $\gamma = 1$ . The probit objective function is

(10) 
$$\mathsf{J}_{\mathrm{p}}^{(n)}(u) = J_{n}^{(\alpha,\tau)}(u) + r_{n} \Phi_{\mathrm{p}}^{(n)}(u;\gamma).$$

where  $r_n = \frac{1}{n}$  in Labeling Model 1 and  $r_n = 1$  in Labeling Model 2. The proof of Proposition 1 in [6] is readily modified to prove the following.

<sup>339</sup> PROPOSITION 6. The objective function  $J_{p}^{(n)}$  is strictly convex.

It is also straightforward to check, by expanding u in the basis given by eigenvectors of  $A^{(n)}$ , that  $J_p^{(n)}$  is coercive. This is proved by establishing that  $J_n^{(\alpha,\tau)}$  is coercive on the orthogonal complement of the constant function. The coercivity in



FIG. 1. The function  $\Psi(\cdot; 1)$ , defined by (8), and its logarithm, which appears in the probit objective function.

the remaining direction is provided by  $\Phi_{\rm p}^{(n)}(u;\gamma)$  using the fact that  $\Omega^+$  and  $\Omega^-$  are nonempty. Consequently  $J_{\rm p}^{(n)}$  has a unique minimizer; Lemma 9 has the proof of the 343 344 continuum analog of this; the proof on a graph is easily reconstructed from this. 345

The probabilistic analogue of the optimization problem for  $J_p^{(n)}$  is as follows. We let  $\nu_0^{(n)}(du;r)$  denote the centred Gaussian with covariance  $C = r_n(A^{(n)})^{-1}$  (with respect to the inner product  $\langle \cdot, \cdot \rangle_{\mu_n}$ ). We assume that the latent variable u is a priori 346 347 348 distributed according to measure  $\nu_0^{(n)}(\mathrm{d} u; r_n)$ . If we then define the likelihood y|u349 through the generative model 350

(11) 
$$y_j = S(u_j + \eta_j)$$

with  $\eta_i \stackrel{\text{iid}}{\sim} N(0, \gamma^2)$  then the posterior probability on u|y is given by 351

(12) 
$$\nu_{\mathbf{p}}^{(n)}(\mathrm{d}u) = \frac{1}{Z_{\mathbf{p}}^{(n)}} e^{-\Phi_{\mathbf{p}}^{(n)}(u;y)} \nu_{0}^{(n)}(\mathrm{d}u;r_{n})$$

with  $Z_{\rm p}^{(n)}$  the normalization to a probability measure. The measure  $\nu_{\rm p}^{(n)}$  has Lebesgue 352 density proportional to  $e^{-r_n^{-1}J_p^{(n)}(u)}$ . 353

3.2. Bayesian Level Set. We now define 354

(13) 
$$\Phi_{\rm ls}^{(n)}(u;\gamma) = \frac{1}{2\gamma^2} \sum_{j \in Z'} |y_j - S(u_j)|^2.$$

The relevant objective function is 355

$$\mathsf{J}_{\rm ls}^{(n)}(u) = J_n^{(\alpha,\tau)}(u) + r_n \Phi_{\rm ls}^{(n)}(u;\gamma).$$

where again  $r_n = \frac{1}{n}$  in Labeling Model 1 and  $r_n = 1$  in Labeling Model 2. We have the following: 356 357

PROPOSITION 7. The infimum of of  $J_{ls}^{(n)}$  is not attained. 358

This follows using the argument introduced in a related context in [28]: assuming 359 that a non-zero minimizer does exist leads to a contradiction upon multiplication of 360 that minimizer by any number less than one; and zero does not achieve the infimum. 361

We modify the generative model (11) slightly to read 362

$$y_j = S(u_j) + \eta_j,$$

where now  $\eta_j \stackrel{\text{iid}}{\sim} N(0, r_n^{-1}\gamma^2)$ . In this case, because the noise is additive, multiplying the objective function by  $r_n$  simply results in a rescaling of the observational noise; 364

multiplication by  $r_n$  does not have such a simple interpretation in the case of probit. As a consequence the resulting Bayesian posterior distribution has significant differences with the probit case: the latent variable u is now assumed a priori to be distributed according to measure  $\nu_0^{(n)}(du; 1)$  Then

(14) 
$$\nu_{\rm ls}^{(n)}({\rm d}u) = \frac{1}{Z_{\rm ls}^{(n)}} e^{-r_n \Phi_{\rm ls}^{(n)}(u;\gamma)} \nu_0^{(n)}({\rm d}u;1)$$

where  $\nu_0^{(n)}$  is the same centred Gaussian as in the probit case. Note that  $\nu_{\rm ls}^{(n)}$  is also the measure with Lebesgue density proportional to  $e^{-J_{\rm ls}^{(n)}(u)}$ .

**3.3. Small Noise Limit.** When the size of the noise on the labels is small, the probit and Bayesian level set approaches behave similarly. More precisely, the measures  $\nu_{\rm p}^{(n)}$  and  $\nu_{\rm ls}^{(n)}$  share a common weak limit as  $\gamma \to 0$ . The following result is given without proof – this is because its proof is almost identical to that arising in the continuum limit setting of Theorem 14(ii) given in the appendix; indeed it is technically easier due to the fully discrete setting. Here  $\Rightarrow$  denotes weak convergence of probability measures.

THEOREM 8. Let  $\nu_0^{(n)}(du)$  denote a Gaussian measure of the form  $\nu_0^{(n)}(du;r)$  for any r, possibly depending on n. Define the set

$$B_n = \{ u \in \mathbb{R}^n \mid y_j u_j > 0 \text{ for each } j \in Z' \}$$

and the probability measure

$$\nu^{(n)}(\mathrm{d}u) = \mathsf{Z}^{-1} \mathbb{1}_{B_n}(u) \nu_0^{(n)}(\mathrm{d}u)$$

where  $Z = \nu_0^{(n)}(B_n)$ . Consider the posterior measures  $\nu_p^{(n)}$  defined in (12) and  $\nu_{ls}^{(n)}$ defined in (14). Then  $\nu_p^{(n)} \Rightarrow \nu^{(n)}$  and  $\nu_{ls}^{(n)} \Rightarrow \nu^{(n)}$  as  $\gamma \to 0$ .

**3.4.** Kriging. Instead of classification, where the sign of the latent variable u is made to agree with the labels, one can alternatively consider regression where u itself is made to agree with the labels [53, 54]. We consider this situation numerically in section 5. Here the objective is to

minimize 
$$\mathsf{J}_{\mathbf{k}}^{(n)}(u) \coloneqq J_{n}^{(\alpha,\tau)}(u)$$
 subject to  $u(x_{j}) = y_{j}$  for all  $j \in Z'$ .

In the continuum setting this minimization is referred to as kriging, and we extend the terminology to our graph based setting. Kriging may also be defined in the case where the constraint is enforced as a soft least squares penalty; however we do not discuss this here.

The probabilistic analogue of this problem can be linked with the original work of Zhu et al [53, 54] which based classification on a centred Gaussian measure with inverse covariance given by the graph Laplacian, conditioned to take the value exactly 1 on labelled nodes where  $y_j = 1$ , and to take the value exactly -1 on labelled nodes where  $y_j = -1$ .

4. Function Space Limits of Graph Based Formulations. In this section we state  $\Gamma$ -limit theorems for the objective functions appearing in the probit algorithm. The proofs are given in the appendix. They rely on arguments which use the fact that we study perturbations of the  $\Gamma$ -limit theorem for the quadratic forms stated in section 2. We also write down formal infinite dimensional formulations of the probit and Bayesian level set posterior distributions, although we do not prove that these limits are attained. We do, however, show that the probit and level set posteriors have a common limit as  $\gamma \rightarrow 0$ , as they do on a finite graph.

401 **4.1. Probit.** Under Labelling Model 1, the natural continuum limit of the 402 probit objective functional is

(15) 
$$\mathsf{J}_{\mathrm{p}}(v) = J_{\infty}^{(\alpha,\tau)}(v) + \Phi_{\mathrm{p},1}(v;\gamma)$$

403 where

(16) 
$$\Phi_{\mathbf{p},1}(v;\gamma) = -\int_{\Omega'} \log(\Psi(y(x)v(x);\gamma)) \,\mathrm{d}\mu(x)$$

for a given measurable function  $y: \Omega' \to \{\pm 1\}$ . For any  $v \in L^2_{\mu}$ ,  $\log(\Psi(y(x)v(x);\gamma))$ is integrable by Corollary 26. The proof of the following theorem is given in the appendix, in section 7.5.

LEMMA 9. Let Assumptions 1–3 hold. For  $\alpha \geq 1$ , consider the functional  $J_{\rm p}$  with Labelling Model 1 defined by (15). Then, the functional  $J_{\rm p}$  has a unique minimizer in  $\mathcal{H}^{\alpha}(\Omega)$ .

<sup>410</sup> *Proof.* Convexity of  $J_p$  follows from the proof of Proposition 1 in [6]. Let  $\bar{v}_+$  and <sup>411</sup>  $\bar{v}_-$  be the averages of v on  $\Omega_+$  and  $\Omega_-$  respectively. Namely let  $\bar{v}_{\pm} = \frac{1}{|\Omega_{\pm}|} \int_{\Omega_{\pm}} v(x) dx$ . <sup>412</sup> Note that

$$\mathsf{J}_{p}(v) \ge J_{\infty}^{(\alpha,\tau)}(v) \ge \lambda_{2}^{\alpha-1} J_{\infty}^{(1,0)}(v) = -\frac{1}{2} \lambda_{2}^{\alpha-1} \int_{\Omega} v \nabla \cdot (\rho^{2} \nabla v) \, \mathrm{d}x \ge \frac{(\rho^{-})^{2} \lambda_{2}^{\alpha-1}}{2} \|\nabla v\|_{L^{2}(\Omega)}^{2}.$$

<sup>413</sup> Using the form of Poincaré inequality given in Theorem 13.27 of [29] implies that

(17) 
$$\mathsf{J}_{\mathrm{p}}(v) \gtrsim \|\nabla v\|_{L^{2}(\Omega)}^{2} \gtrsim \int_{\Omega} |v - \bar{v}_{+}|^{2} + |v - \bar{v}_{-}|^{2} \,\mathrm{d}x.$$

<sup>414</sup> The convexity of  $\Phi_{p,1}(v;\gamma)$  implies that

$$\Phi_{\mathrm{p},1}(v;\gamma) \ge -\log(\Psi(\bar{v}_{+});\gamma)\mu(\Omega_{+}) - \log(\Psi(-\bar{v}_{-});\gamma)\mu(\Omega_{-})$$

<sup>415</sup> Using that  $\lim_{s\to\infty} -\log(\Psi(s;\gamma)) = \infty$  we see that a bound on  $\Phi_{p,1}(v;\gamma)$  provides a <sup>416</sup> lower bound on  $\bar{v}_+$  and an upper bound on  $\bar{v}_-$ . To see this let  $\Theta$  be the inverse of <sup>417</sup>  $s \mapsto -\log(\Psi(s;\gamma))$ . The preceding shows that

$$\bar{v}_{+} \ge \Theta\left(\frac{\Phi_{\mathrm{p},1}(v;\gamma)}{\mu(\Omega_{+})}\right) \ge \Theta\left(\frac{\mathsf{J}_{\mathrm{p}}(v)}{\mu(\Omega_{+})}\right) \quad \text{and} \quad \bar{v}_{-} \le -\Theta\left(\frac{\Phi_{\mathrm{p},1}(v;\gamma)}{\mu(\Omega_{-})}\right) \le -\Theta\left(\frac{\mathsf{J}_{\mathrm{p}}(v)}{\mu(\Omega_{-})}\right)$$

Let  $c = \max\left\{-\Theta\left(\frac{J_{p}(v)}{\mu(\Omega_{+})}\right), -\Theta\left(\frac{J_{p}(v)}{\mu(\Omega_{-})}\right), 0\right\}$ . Then  $\bar{v}_{+} \ge -c$  and  $\bar{v}_{-} \le c$ . Using that, for any  $a \in \mathbb{R}, v^{2} \le 2|v-a|^{2} + 2a^{2}$ , we obtain

$$\begin{split} \int_{\Omega} v^2(x) \, \mathrm{d}x &\leq \int_{\{v(x) \leq -c\}} v^2(x) \, \mathrm{d}x + \int_{\{v(x) \geq c\}} v^2(x) \, \mathrm{d}x + c^2 |\Omega| \\ &\leq 2 \int_{\{v(x) \leq -c\}} |v + c|^2 + c^2 \, \mathrm{d}x + 2 \int_{\{v(x) \geq c\}} |v - c|^2 + c^2 \, \mathrm{d}x + c^2 |\Omega| \\ &\leq 5c^2 |\Omega| + 2 \int_{\{v(x) \leq -c\}} |v - \bar{v}_+|^2 \, \mathrm{d}x + 2 \int_{\{v(x) \geq c\}} |v - \bar{v}_-|^2 \, \mathrm{d}x \\ &\lesssim c^2 |\Omega| + \mathcal{J}_{\mathbf{p}}(v). \end{split}$$

<sup>418</sup> Then  $||v||_{L^2}$  is bounded by a function of  $J_p(v)$  and  $\Omega$ .

<sup>419</sup> Combining with (17) implies that a function of  $J_p(v)$  bounds  $||v||^2_{\mathcal{H}^{\alpha}(\Omega)}$  which <sup>420</sup> establishes the coercivity of  $J_p$ . The functional  $J_p$  is weakly lower-somicontinuous in <sup>421</sup>  $\mathcal{H}^{\alpha}$ , due to convexity of both  $J_{\infty}^{(\alpha,\tau)}$  and  $\Phi_{p,1}$ . Thus the direct method of the calculus <sup>422</sup> of variations proves that  $J_p$  has a unique minimizer in  $\mathcal{H}^{\alpha}(\Omega)$ .

<sup>423</sup> The following theorem is proved in section 7.5.

THEOREM 10. Let the assumptions of Labelling Model 1 and Theorem 1 hold. Then, with probability one, any sequence of minimizers  $v_n$  of  $J_p^{(n)}$  converge in  $TL^2$  to  $v_{\infty}$ , the unique minimizer of  $J_p$  in  $L^2_{\mu}$ , and furthermore  $\lim_{n\to\infty} J_p^{(n)}(v_n) = J_p(v_{\infty}) =$ 

427  $\min_{v \in L^2_{\mu}} \mathsf{J}_{p}(v).$ 

The analogous result under Labelling Model 2, i.e. convergence of minimizers, is an open question. In this case the natural continuum limit of the probit objective functional is

(18) 
$$\mathsf{J}_{\mathrm{p}}(v) = J_{\infty}^{(\alpha,\tau)}(v) + \Phi_{\mathrm{p},2}(v;\gamma)$$

431 where

(19) 
$$\Phi_{\mathbf{p},2}(v;\gamma) = -\sum_{j \in Z'} \log(\Psi(y(x_j)u(x_j);\gamma)$$

for a given measurable function  $y: \Omega' \to \{\pm 1\}$ . When  $\alpha \leq \frac{d}{2}$  this limiting model 432 is not well-posed. In particular the regularity of the functional is not sufficient to 433 impose pointwise data. More precisely, when  $\alpha \leq \frac{d}{2}$  then there exists a sequence of 434 smooth functions  $v_k \in C^{\infty}(\Omega)$  such that  $\lim_{k\to\infty} J_p(v_k) = 0$ . In particular when  $\alpha < \frac{d}{2}$ , 435 consider a smooth, compactly supported, mollifier  $\xi$ , with  $\xi(0) > 0$  and define  $v_k(x)$ 436  $c_k \sum_{i=1}^N y(x_i) \xi_{1/k}(x-x_i)$  where  $c_k \to \infty$  sufficiently slowly. Then  $\Phi_{p,2}(v_k;\gamma) \to 0$  as 437  $k \to \infty$  and, by a simple scaling argument (for appropriate  $c_k$ ),  $J_{\infty}^{(\alpha,\tau)}(v_k) \to 0$  as 438  $k \to \infty$ . Another way to see that the problem is not well defined is that the functions 439 in  $\mathcal{H}^{\alpha}(\Omega)$  (which is the natural space to consider  $J_{p}$  on) are not continuous in general 440 and evaluating  $\Phi_{p,2}(v;\gamma)$  is not well defined. 441

<sup>442</sup> When  $\alpha > \frac{d}{2}$  the existence of minimizers of (18) in  $\mathcal{H}^{\alpha}(\Omega)$  is established by the <sup>443</sup> direct method of the calculus of variations using the convexity of  $J_p$  and the fact that, <sup>444</sup> by Lemma 3,  $\mathcal{H}^{\alpha}$  continuously embeds into a set of Hölder continuous functions.

For  $\alpha > \frac{d}{2}$  we believe that the minimizers of  $J_p^n$  of Labelling Model 2 converge to minimizers of (18) in an appropriate regime, but the situation is more complicated than for Labelling Model 1: under Labelling Model 2 (5) is no longer a sufficient condition on the scaling of  $\varepsilon$  with n for the convergence to hold. Thus if  $\varepsilon \to 0$  too slowly the problem degenerates. In particular in the following theorem we identify the asymptotic behavior of minimizers of  $J_p$  both when  $\alpha < \frac{d}{2}$ , and if  $\alpha > \frac{d}{2}$  but  $\varepsilon \to 0$ too slowly.

The proof of the following may be found in section 7.6. The theorem is similar in spirit to Proposition 2.2(ii) in [38] where a similar phenomenon was discussed for the *p*-Laplacian regularized semi-supervised learning. We also mention that the PDE approach to a closely related *p*-Laplacian problem was recently introduced by Calder [12].

<sup>457</sup> THEOREM 11. Let the assumptions of Labelling Model 2, and Theorem 1 hold. <sup>458</sup> If  $\alpha > \frac{d}{2}$ ,  $\tau > 0$ , and

(20) 
$$\varepsilon_n n^{\frac{1}{2\alpha}} \to \infty$$
 as  $n \to \infty$ 

<sup>459</sup> or if  $\alpha < \frac{d}{2}$  then, with probability one, the sequence of minimizers  $v_n$  of  $J_p^{(n)}$  converge <sup>460</sup> to 0 in  $TL^2$  as  $n \to \infty$ . That is, the minimizers of  $J_p^{(n)}$  converge to the minimizer of <sup>461</sup>  $J_{\infty}^{(\alpha,\tau)}$  with the information about the labels being lost in the limit.

462 Remark 12. We believe, but do not have a proof, that for  $\alpha > \frac{d}{2}$  and  $\tau > 0$ , if

$$\varepsilon_n n^{\frac{1}{2\alpha}} \to 0 \qquad \text{as } n \to \infty$$

then, with probability one, any sequence of minimizers  $v_n$  of  $J_p^{(n)}$  is sequentially compact in  $TL^2$  with  $\lim_{n\to\infty} J_p^{(n)}(v_n) = \min_{v\in L^2_{\mu}} J_p(v)$  given by (18), (19). If this holds then, under Labelling Model 2,  $J_p^{(n)}(u)$  converges in an appropriate sense to a limiting objective function  $J_p(u)$ . Our numerical results support this conjecture.

It is also of interest to consider the limiting probability distributions which arise under the two labelling models. Under **Labelling Model 2** this density has, in physicist's notation, "Lebesgue density"  $\exp(-J_p(u))$ . Under **Labelling Model 1**, however, we have shown that  $J_p^{(n)}(u)$  converges in an appropriate sense to a limiting objective function  $J_p(u)$  implying that (again in physicist's notation)  $\exp(-r_n^{-1}J_p^{(n)}(u)) \approx$  $\exp(-nJ_p(u))$ . Thus under **Labelling Model 1** the posterior probability concentrates on a Dirac measure at the minimizer of  $J_p(u)$ .

Based on this remark, the natural continuum probability limit concerns Labelling Model 2. The posterior probability is then given by

(21) 
$$\nu_{p,2}(du) = \frac{1}{Z_{p,2}} e^{-\Phi_{p,2}(u;\gamma)} \nu_0(du)$$

where  $\nu_0$  is the centred Gaussian with covariance C given in Theorem 4 and  $\Phi_{p,2}$  is given by (19). Since we require pointwise evaluation to make sense of  $\Phi_{p,2}(u;\gamma)$  we, in general, require  $\alpha > d$ ; however Proposition 5 gives conditions under which  $\alpha > \frac{d}{2}$ will suffice. We will also consider the probability measure  $\nu_{p,1}$  defined by

(22) 
$$\nu_{p,1}(du) = \frac{1}{Z_{p,1}} e^{-\Phi_{p,1}(u;\gamma)} \nu_0(du)$$

where  $\Phi_{p,1}$  is given by (16). The function  $\Phi_{p,1}(u;\gamma)$  is defined in an  $L^2_{\mu}$  sense and 480 thus we require only  $\alpha > \frac{d}{2}$  - see Theorem 4. Note, however, that this is not the 481 limiting probability distribution that we expect for Labelling Model 1 with the 482 parameter choices leading to Theorem 10 since the argument above suggests that this 483 will concentrate on a Dirac. However we include the measure  $\nu_{p,1}$  in our discussions 484 because, as we will show, it coincides with the analogous Bayesian level set measure 485  $\nu_{\rm ls,1}$  (defined below) in the small observational noise limit. Since  $\nu_{\rm ls,1}$  can be obtained 486 by a natural scaling of the graph algorithm, which does not concentrate on Dirac, 487 the relationship between  $\nu_{p,1}$  and  $\nu_{ls,1}$  is of interest as they are both, for small noise, 488 relaxations of the same limiting object. 489

**4.2.** Bayesian Level Set. We now study probabilistic analogues of the Bayesian level set method, again using the measure  $\nu_0$  which is the centred Gaussian with covariance C given in Theorem 4 for some  $\alpha > \frac{d}{2}$ . Note that, from equation (13), for

## Labelling Model 1,

$$r_n \Phi_{ls}^{(n)}(u;\gamma) = \frac{1}{2\gamma^2} \frac{1}{n} \sum_{j \in Z'} |y(x_j) - S(u(x_j))|^2$$
$$\approx \int_{\Omega'} \frac{1}{2\gamma^2} |y(x) - S(u(x))|^2 d\mu(x)$$
$$\coloneqq \Phi_{ls,1}(u;\gamma)$$

<sup>490</sup> by a law of large numbers type argument of the type underlying the proof of Theorem<sup>491</sup> 10.

Recall that, from the discussion following Proposition 7, this scaling corresponds to employing the finite dimensional Baysian level set model with observational variance  $\gamma^2 n$  so that the variance per observation is constant. Then the natural limiting probability measure is, in physicists notation,  $\exp(-J_{ls}(u))$  where

$$\mathsf{J}_{\mathrm{ls}}(u) = J_{\infty}^{(\alpha,\tau)}(u) + \Phi_{\mathrm{ls},1}(u;\gamma)$$

<sup>496</sup> Expressed in terms of densities with respect to the Gaussian prior this gives

(23) 
$$\nu_{\mathrm{ls},1}(\mathrm{d}u) = \frac{1}{Z_{\mathrm{ls},1}} e^{-\Phi_{\mathrm{ls},1}(u;\gamma)} \nu_0(\mathrm{d}u).$$

Since  $\Phi_{ls,1}(u;\gamma)$  makes sense in  $L^2_{\mu}$  we equire only  $\alpha > \frac{d}{2}$ . The measure  $\nu_{ls,1}$  is the natural analogue of the finite dimensional measure  $\nu_{ls}^{(n)}$  under this label model. Under **Labelling Model 2** we take  $r_n = 1$ . We obtain a measure  $\nu_{ls,2}$  in the form (23) found by replacing  $\nu_{ls,1}$  by  $\nu_{ls,2}$  and  $\Phi_{ls,1}$  by

(24) 
$$\Phi_{\mathrm{ls},2}(u;\gamma) \coloneqq \sum_{j \in Z'} \frac{1}{2\gamma^2} |y(x_j) - S(u(x_j))|^2.$$

In this case the observational variance is not-rescaled by n since the total number of labels is fixed. Since we require pointwise evaluation to make sense of  $\Phi_{\rm ls,2}(u;\gamma)$  we, in general, require  $\alpha > d$ ; however Proposition 5 gives conditions under which  $\alpha > \frac{d}{2}$ will suffice.

Remark 13. Note that  $J_{ls}^{(n)}$  and  $J_{ls}$  cannot be connected via Γ-convergence. Indeed, if  $J_{ls} = \Gamma - \lim_{n \to \infty} J_{ls}^{(n)}$  then  $J_{ls}$  would be lower semi-continuous [10]. When  $\tau > 0$  compactness of minimizers follows directly from the compactness property of the quadratic forms  $J_n^{(\alpha,\tau)}$ , see Theorem 1. Now since compactness of minimizers plus lower semi-continuity implies existence of minimizers then the above reasoning implies there exists minimizers of  $J_{ls}$ . But as in the discrete case, Proposition 7, multiplying any u by a constant less than one leads to a smaller value of  $J_{ls}$ . Hence the infimum cannot be achieved. It follows that  $J_{ls} \neq \Gamma - \lim_{n \to \infty} J_{ls}^{(n)}$ .

**4.3. Small Noise Limit.** As for the finite graph problems, the labeled data can be viewed as arising from different generative models. In the probit formulation, the generative models for the labels are given by

$$y(x) = S(u(x) + \eta(x)), \quad \eta \sim N(0, \gamma^2 I),$$
$$y(x_j) = S(u(x_j) + \eta_j), \quad \eta_j \stackrel{\text{iid}}{\sim} N(0, \gamma^2).$$
15

for Labelling Model 1, Labelling Model 2 respectively; S is the sign function. The functionals  $\Phi_{p,1}$ ,  $\Phi_{p,2}$  then arise as the negative log-likelihoods from these models. Similarly, in the Bayesian level set formulation the generative models are given by

$$y(x) = S(u(x)) + \eta(x), \quad \eta \sim N(0, \gamma^2 I),$$
  
$$y(x_j) = S(u(x_j)) + \eta_j, \quad \eta_j \stackrel{\text{iid}}{\sim} N(0, \gamma^2).$$

<sup>513</sup> leading to the functionals  $\Phi_{ls,1}$ ,  $\Phi_{ls,2}$ .

We show that in the zero noise limit the Bayesian level set and probit posterior 514 distributions coincide. However for  $\gamma > 0$  they differ: note, for example, that the 515 probit model enforces binary data, whereas the Bayesian level set model does not. 516 It has been observed that the Bayesian level set posterior can be used to produce 517 similar quality classification to the Ginzburg-Landau posterior, at significantly lower 518 computational cost [18]. The small noise limit is important for two reasons: firstly 519 in many applications labelling is very accurate and considering the zero noise limit is 520 therefore instructive; secondly recent work [5] shows that the zero noise limit provides 521 useful information about the efficiency of algorithms applied to sample the posterior 522 distribution and, in particular, constants derived from the zero noise limit appear 523 in lower bounds on average acceptance probability and mean square jump in such 524 algorithms. 525

<sup>526</sup> Proof of the following is given in section 7.7.

527 THEOREM 14.

5

(i) Let Assumptions 2-3 hold, and assume that  $\alpha > d$ . Let the assumptions of Labelling Model 1 hold. Define the set

$$B_{\infty,1} = \{ u \in C(\Omega; \mathbb{R}) \mid y(x)u(x) > 0 \text{ for a.e. } x \in \Omega' \}$$

and the probability measure

$$\nu_1(\mathrm{d}u) = \mathsf{Z}^{-1} \mathbb{1}_{B_{\infty,1}}(u) \nu_0(\mathrm{d}u)$$

where  $Z = \nu_0(B_{\infty,1})$ . Consider the posterior measures  $\nu_{p,1}$  defined in (22) and  $\nu_{ls,1}$  defined in (23). Then  $\nu_{p,1} \Rightarrow \nu_1$  and  $\nu_{ls,1} \Rightarrow \nu_1$  as  $\gamma \to 0$ . (i) Let Assumptions 2-3 hold, and assume that  $\alpha > d$ . Let the assumptions of

<sup>532</sup> (ii) Let Assumptions 2-3 hold, and assume that  $\alpha > d$ . Let the assumptions of <sup>533</sup> Labelling Model 2 hold. Define the set

$$B_{\infty,2} = \{ u \in C(\Omega; \mathbb{R}) \mid y(x_j) \mid u(x_j) > 0 \text{ for each } j \in Z' \}$$

and the probability measure

$$\nu_2(\mathrm{d}u) = \mathsf{Z}^{-1} \mathbb{1}_{B_{\infty,2}}(u) \nu_0(\mathrm{d}u)$$

where 
$$\mathsf{Z} = \nu_0(B_{\infty,2})$$
. Then  $\nu_{\mathrm{p},2} \Rightarrow \nu_2$  and  $\nu_{\mathrm{ls},2} \Rightarrow \nu_2$  as  $\gamma \to 0$ .

Remark 15. The assumption that  $\alpha > d$  in both parts of the above theorem can be relaxed to  $\alpha > d/2$  if the conclusions of Proposition 5 are satisfied.

4.4. Kriging. One can define kriging in the continuum setting [47] analogously to the discrete setting; we consider this numerically in section 5. In the case of Labelling Model 2, the limiting problem is to

minimize 
$$J_k(u) \coloneqq J_{\infty}^{(\alpha,\tau)}(u)$$
 subject to  $u(x_i) = y_i$  for all  $j \in Z'$ .

540 Kriging may also be defined for Labelling Model 1 and without the hard constraint

541 in the continuum setting, but we do not discuss either of these scenarios here.



FIG. 2. The cross sections of the data densities  $\rho_h$  we consider in subsection 5.1.

5. Numerical Illustrations. In this section we describe the results of numerical 542 experiments which illustrate or extend the developments in the preceding sections. 543 In section 5.1 we study the effect of the geometry of the data on the classification 544 problem, by studying an illustrative example in dimension d = 2. Section 5.2 studies 545 how the relationship between the length-scale  $\epsilon$  and the graph size n affects limiting 546 behaviour. In section 5.3 we study graph based kriging. Finally, in section 5.4, we 547 study continuum problems from the Bayesian perspective, studying the quantification 548 of uncertainty in the resulting classification. 549

5.1. Effect of Data Geometry on Classification. We study how the ge-550 ometry of the data affects the classification under Labelling Model 1, using the 551 continuum probit model. Let  $\Omega = (0,1)^2$ . We first consider a uniform distribution  $\rho$ 552 on the domain, and choose  $\Omega_+, \Omega_-$  to be balls of radius 0.05 centred at (0.25,0.25), 553 (0.75, 0.75) respectively. The decision boundary is then naturally the perpendicular 554 bisector of the line segment joining the centers of these balls. We then modify  $\rho$  by 555 introducing a channel of increasing depth in  $\rho$  dividing the domain in two vertically, 556 and look at how this affects the decision boundary. Specifically, given  $h \in [0,1]$  we 557 define  $\rho_h$  to be constant in the y-direction, and assume the cross-sections in the x-558 direction are as shown in Figure 2, so that the channel has depth 1 - h. In order to 559 numerically estimate the continuum probit minimizers, we construct a finite-difference 560 approximation to each  $\mathcal{L}$  on a uniform grid of 65536 points, which then provides an 561 approximation to  $\mathcal{A}$ . The objective function  $J_p^{(\infty)}$  is then minimized numerically using 562 the linearly-implicit gradient flow method described in [6], Algorithm 4. 563

We consider both the effect of the channel depth parameter h and the parameter 564  $\alpha$  on the classification; we fix  $\tau = 10$  and  $\gamma = 0.01$ . In Figure 3 we show the minimizers 565 arising from 5 different choices of h and  $\alpha = 1, 2, 3$ . As the depth of the channel is in-566 creased, the minimizers begin to develop a jump along the channel. As  $\alpha$  is increased, 567 the minimizers become less localized around the labelled regions, and the jump along 568 the channel becomes sharper as a result. Note that the scale of the minimizers de-569 creases as  $\alpha$  increases. This could formally be understood from a probabilistic point 570 of view: under the prior we have  $\mathbb{E} \| u \|_{L^2}^2 = \operatorname{Tr}(\mathcal{A}^{-1}) \asymp \tau^{-2\alpha}$ , and so a similar scaling 571 may be expected to hold for the MAP estimators. In Figure 4 we show the sign of 572 each minimizer in Figure 3 to illustrate the resulting classifications. As the depth of 573 the channel is increased, the decision boundary moves continuously from the diagonal 574 to the vertical bisector of the domain, with the transitional boundaries appearing al-575 most as a piecewise linear combination of both boundaries. We also see that, despite 576 the minimizers themselves differing significantly for different  $\alpha$ , the classifications are 577 almost invariant with respect to  $\alpha$ . 578



FIG. 3. The minimizers of the functional  $J_p^{(\infty)}$  for different values of h and  $\alpha$ , as described in subsection 5.1.

579 5.2. Localization Bounds for Kriging and Probit. We study how the rate 580 at which the localization parameter  $\varepsilon$  decreases when the number of data points n581 is increased affects convergence to the continuum limits. We consider Labelling 582 model 2 using both the kriging and probit models; this serves to illustrate the result 583 of Theorem 11, motivate Remark 12, and provide a relation to the results of [38].

<sup>584</sup> We work on the domain  $\Omega = (0,1)^2$  and take a uniform data distribution  $\rho$ . In <sup>585</sup> all cases we fix two datapoints which we label with opposite signs, and sample the <sup>586</sup> remaining n-2 datapoints. For kriging we consider the situation where the data <sup>587</sup> is viewed as noise-free so that the label values are interpolated. We calculate the <sup>588</sup> minimizer  $u_n$  of  $J_k^{(n)}$  numerically via the closed form solution

$$u_n = A^{(n),-1} R^* (R A^{(n),-1} R^*)^{-1} y,$$

where  $R \in \mathbb{R}^{2 \times n}$  is the mapping taking vectors to their values at the labelled points. In order to numerically estimate the continuum minimizer u of  $J_{k}^{(\infty)}$ , we construct a finite-difference approximation to  $\mathcal{L}$  on a uniform grid of 65536 points. This leads to an approximation  $\hat{\mathcal{A}}$  to  $\mathcal{A}$ , from which we again use the closed form solution to compute  $\hat{u} \approx u$ :

$$\hat{u} = \hat{\mathcal{A}}^{-1}\hat{R}^*(\hat{R}\hat{\mathcal{A}}^{-1}\hat{R}^*)^{-1}y,$$

where  $\hat{R} \in \mathbb{R}^{2 \times 65556}$  takes discrete functions to their values at the labelled points.

In Figure 5 (left) we show how the  $L^2_{\mu_n}$  error between  $u_n$  and  $\hat{u}$  varies with respect to  $\varepsilon$  for increasing values of n. All errors are averaged over 200 realizations of the



FIG. 4. The sign of minimizers from Figure 3, showing the resulting classification.

unlabelled datapoints, and we consider 100 uniformly spaced values of  $\varepsilon$  between 0.005 597 and 0.5. We see that  $\varepsilon$  must belong to a 'sweet-spot' in order to make the error small 598 - if  $\varepsilon$  is too small or too large convergence doesn't occur. The right hand side of the 599 figure shows how these lower and upper bounds vary with n; the bounds are defined 600 numerically as the points where the second derivative of the error curve changes sign. 601 The rates are in agreement with the results and conjectures up to logarithmic terms, 602 although the sharp bounds are not obtained – we see that the lower bounds are larger 603 than  $\mathcal{O}(n^{-\frac{1}{2}})$ , and the upper bounds are smaller than  $\mathcal{O}(n^{-\frac{1}{2\alpha}})$ . It is possible that 604 the sharp bounds may be approached in a more asymptotic (and computationally 605 infeasible) regime. 606

Similarly, we note that the minimum error for  $\alpha = 2$  in Figure 5 decreases very slowly in the range of n we considered. This again indicates that we are not yet in the asymptotic regime at n = 1600. Further experiments (not included) for larger values of n show that the minimum error does converge as  $n \to \infty$  as expected.

For the probit model we take  $\gamma = 0.01$  and use the same gradient flow algorithm as in subsection 5.1 for both the continuum and discrete minimizers. Figure 6 shows the errors, analogously to Figure 5. Note that the errors are plotted on logarithmic axes here, as unlike the kriging minimizers, there is no restriction for the minimizers to be on the same scale as the labels. We see that the same trend is observed in terms of requiring upper and lower bounds on  $\varepsilon$ , and a shift of the error curves towards the left as n is increased.



FIG. 5. (Left) The  $L^2_{\mu_n}$  error between discrete minimizers and continuum minimizers of the kriging model versus localization parameter  $\varepsilon$ , for different values of n. (Right) The upper and lower bounds for  $\varepsilon(n)$  to provide convergence. The slopes of the lines of best fit provide estimates of the rates.

5.3. Extrapolation on Graphs. We consider the problem of smoothly extend-618 ing a sparsely defined function on a graph to the entire graph. Such extrapolation was 619 studied in [37], and was achieved via the use of a weighted nonlocal Laplacian. We 620 use the kriging model with Labelling Model 2, labelling two points with opposite 621 signs, and setting  $\gamma = 0$ . We fix a set of datapoints  $\{x_j\}_{j=1}^n$ , n = 1600, drawn from the uniform density on the domain  $\Omega = (0,1)^2$ . We fix  $\tau = 1$  and look at how the 622 623 smoothness of minimizers of the kriging functional  $J_k^{(n)}$  varies with  $\alpha$ . The minimizers are computed directly from the closed form solution, as in subsection 5.2. When 624 625  $\alpha > d/2$  we choose  $\varepsilon$  to approximately minimize the  $L^2_{\mu_n}$  errors between the discrete 626



FIG. 6. (Left) The  $L^2_{\mu_n}$  error between discrete minimizers and continuum minimizers of the probit model versus localization parameter  $\varepsilon$ , for different values of n. (Right) The upper and lower bounds for  $\varepsilon(n)$  to provide convergence. The slopes of the lines of best fit provide estimates of the rates.

and continuum solutions (since the continuum solution is non-trivial). When  $\alpha \leq d/2$ a representative  $\varepsilon$  is chosen which is approximately twice the connectivity radius. The minimizers are shown in Figure 7 for  $\alpha = 0.5, 1.0, 1.5, 2.0$ . Spikes are clearly visible for  $\alpha \leq d/2 = 1$ : the requirement for  $\alpha > d/2$  to avoid spikes appears to be essential.

**5.4. Bayesian Level Set for Sampling.** We now turn to the problem of sampling the conditioned continuum measures introduced in subsections 4.1 and 4.2, specifically their common  $\gamma \rightarrow 0$  limit. From this sampling we can, for example, calculate the mean of the classification, which may be used to define a measure of uncertainty of the classification at each point. This is because, for binary random





FIG. 7. The extrapolation of a sparsely defined function on a graph using the kriging model, for various choices of parameter  $\alpha$ .

variables, the mean determines the variance. Knowing the uncertainty in classifica tion has great potential utility, for example in active learning in guiding where to
 place resources in labelling in order to reduce uncertainty.

We fix  $\Omega = (0,1)^2$ . The data distribution  $\rho$  is shown in Figure 8; it is constructed 639 as a continuum analogue of the two moons distribution [49], with the majority of 640 its mass concentrated on two curves. The contrast ratio in the sampling density 641  $\rho$  is approximately 100:1 between the values on and off of the curves. The resulting 642 operator  $\mathcal{L}$  contains significant clustering information: in Figure 8 we show the second 643 eigenfunction of  $\mathcal{L}$ , termed the Fiedler vector in analogy with second eigenvector of the 644 graph Laplacian. The sign of this function provides a good estimate for the decision 645 boundary in an unsupervised context. We use Labelling Model 2, labelling a single 646 point on each curve with opposing signs as indicated by  $\bullet$  and  $\circ$  in Figure 8. 647

<sup>648</sup> Sampling is performed using the preconditioned Crank-Nicolson MCMC algo-<sup>649</sup> rithm [14], which has favourable dimension-independent statistical properties, as



FIG. 8. (Left) The data distribution  $\rho$  used in the MCMC experiments, and the locations of the two labelled datapoints. (Right) The second eigenfunction of the operator  $\mathcal{L}$  corresponding to  $\rho$ .

demonstrated in [19] in the graph-based setting of relevance here. We consider three choices of  $\alpha > d/2$ , and two choices of inverse length-scale parameter  $\tau$ . In general we require  $\alpha > d$  for the measure  $\nu_2$  in Theorem 14 to be well-defined. However numerical evidence suggests that the conclusions of Proposition 5 are satisfied with this choice of  $\rho$ , implying that we may make use of Remark 15 and that  $\alpha > \frac{d}{2}$  suffices. The operator  $\mathcal{L}$  is discretized using a finite difference method on a square grid of 40000 points, and sampling is performed on the span of its first 500 eigenfunctions.

In Figure 9 we show the mean of the sign of samples on the left hand side, for each 657 choice of  $\alpha$ , after fixing  $\tau = 1$ . Note that uncertainty is greater the further the values of 658 the mean are from ±1: specifically we have that  $\operatorname{Var}(S(u(x)) = 1 - [\mathbb{E}(S(u(x)))]^2)$ . We 659 see that the classification on the curves where the data concentrates is fairly certain, 660 whereas classification away from the curves is uncertain; furthermore the certainty 661 increases away from the curves slightly as  $\alpha$  is increased. Samples S(u) are also 662 shown in the same figure; the uncertainty away from the curves is illustrated also by 663 these samples. 664

In Figure 10 we show the same results, but with the choice  $\tau = 0.2$  so that samples possess a longer length scale. The classification certainty now propagates away from the curves more easily. The effect of the asymmetry of the labelling is also visible in the mean for the case  $\alpha = 4$ : uncertainty is higher in the bottom-left corner than the top-left corner.

Since the prior on the latent random field u may be difficult to ascertain in applications, the sensitivity of the classification on the choice of the parameters  $\alpha$ ,  $\tau$  indicates that it could be wise to employ hierarchical Bayesian methods to learn appropriate values for them along with the latent field u. Dimension robust MCMC methods are available to sample such hierarchical distributions [13], and application to classification problems are shown in that paper.

6. Conclusions. In this paper we have studied large graph limits of semisupervised learning problems in which smoothness is imposed via a shifted graph Laplacian, raised to a power. Both optimization and Bayesian approaches have been considered. To keep the exposition manageable in length we have confined our attention to the unnormalized graph Laplacian. However, one may instead choose to work with the normalized graph Laplacian  $L = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$ , in place of L = D - W. In



FIG. 9. (Left) The mean  $\mathbb{E}(S(u))$  of the classification arising from the conditioned measure  $\nu_2$ . (Right) Examples of samples S(u) where  $u \sim \nu_2$ . Here we choose  $\tau = 1$ .

the normalized case the continuum PDE operator is given by

$$\mathcal{L}u = -\frac{1}{\rho^{3/2}} \nabla \cdot \left(\rho^2 \nabla \left(\frac{u}{\rho^{1/2}}\right)\right)$$

with no flux boundary conditions:  $\nabla(\frac{u}{\rho^{1/2}}) \cdot \nu = 0$  on  $\partial\Omega$ , where  $\nu$  is the outside unit normal vector to  $\partial\Omega$ . Theorems 1, 10 and 14 generalize in a straightforward way to such a change in the graph Laplacian.

Future directions stemming from the work in this paper include: (i) providing a limit theorem for probit MAP estimators under Labelling Model 2; (ii) providing limit theorems for the Bayesian probability distributions considered, using the machinery introduced in [19, 20]; (iii) using the limiting problems in order to analyze and quantify efficiency of algorithms on large graphs; (iv) invoking specific sources of data and studying the effectiveness of PDE limits in comparison to non-local limits.

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FIG. 10. (Left) The mean  $\mathbb{E}(S(u))$  of the classification arising from the conditioned measure  $\nu_2$ . (Right) Examples of samples S(u) where  $u \sim \nu_2$ . Here we choose  $\tau = 0.2$ .

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700		REFERENCES
701	[1]	H. ABELS, Short lecture notes: Interpolation theory and function spaces, 2011, http://www.
702		uni-r.de/Fakultaeten/nat_Fak_I/abels/SkriptInterpolationstheorieSoSe11.pdf.
703	[2]	M. ABRAMOWITZ AND I. A. STEGUN, Handbook of mathematical functions with formulas,
704		graphs, and mathematical tables, vol. 55 of National Bureau of Standards Applied Math-
705		ematics Series, For sale by the Superintendent of Documents, U.S. Government Printing
706		Office, Washington, D.C., 1964.
707	[3]	M. BELKIN AND P. NIYOGI, Laplacian eigenmaps and spectral techniques for embedding and
708		clustering, in Advances in neural information processing systems, 2002, pp. 585–591.
709	[4]	A. L. BERTOZZI AND A. FLENNER, Diffuse interface models on graphs for classification of high
710		dimensional data, Multiscale Modeling & Simulation, 10 (2012), pp. 1090–1118.
711	[5]	A. L. BERTOZZI, X. LUO, O. PAPASPILIOPOULOS, AND A. M. STUART, Scalable and robust sam-
712		pling methods for bayesian graph-based semi-supervised learning, In preparation, (2018).
713	[6]	A. L. BERTOZZI, X. LUO, A. M. STUART, AND K. C. ZYGALAKIS, Uncertainty quantification in
714		the classification of high dimensional data, arXiv preprint arXiv:1703.08816, (2017).
715	[7]	C. BISHOP, Pattern recognition and machine learning (information science and statistics), 1st
716		edn. 2006. corr. 2nd printing edn, Springer, New York, (2007).
717	[8]	A. BLUM AND S. CHAWLA, Learning from labeled and unlabeled data using graph mincuts, tech.
718		report, CMU Tech Report, 2001.
719	[9]	Y. BOYKOV, O. VEKSLER, AND R. ZABIH, Fast approximate energy minimization via graph cuts,

- T20 IEEE Transactions on pattern analysis and machine intelligence, 23 (2001), pp. 1222–1239.
- <sup>721</sup> [10] A. BRAIDES, Γ-Convergence for Beginners, Oxford University Press, Oxford, 2002.
- [11] M. BURGER AND S. OSHER, A survey on level set methods for inverse problems and optimal
   design, Europ. J. Appl. Math., 16 (2005), pp. 263–301.
- [12] J. CALDER, The game theoretic p-Laplacian and semi-supervised learning with few labels, arXiv
   preprint arXiv:1711.10144, (2017).
- [13] V. CHEN, M. M. DUNLOP, O. PAPASILIOPOULOS, AND A. M. STUART, Robust MCMC sampling
   with non-Gaussian and hierarchical priors in high dimensions. In Preparation.
- [14] S. L. COTTER, G. O. ROBERTS, A. M. STUART, AND D. WHITE, MCMC methods for functions: modifying old algorithms to make them faster., Statistical Science, 28 (2013), pp. 424–446.
   [15] R. CRISTOFERI AND M. THORPE, Large data limit for a phase transition model with the p-
- Laplacian on point clouds, arxiv preprint arXiv:1802.08703, (2018).
- <sup>732</sup> [16] G. DAL MASO, An Introduction to  $\Gamma$ -Convergence, Springer, 1993.
- [17] M. DASHTI AND A. M. STUART, *The Bayesian approach to inverse problems*, in Handbook of
   Uncertainty Quantification, Springer, 2016, p. arxiv preprint arXiv:1302.6989.
- [18] M. DUNLOP, C. ELLIOTT, V. HOANG, AND A. STUART, Bayesian formulations of multidimensional barcode inversion. arXiv preprint arXiv:1706.01960.
- [19] N. GARCÍA TRILLOS, Z. KAPLAN, T. SAMAKHOANA, AND D. SANZ-ALONSO, On the consistency
   of graph-based Bayesian learning and the scalability of sampling algorithms, arXiv preprint
   arXiv:1710.07702, (2017).
- [20] N. GARCÍA TRILLOS AND D. SANZ-ALONSO, Continuum limit of posteriors in graph Bayesian
   *inverse problems*, arXiv preprint arXiv:1706.07193, (2017).
- [21] N. GARCÍA TRILLOS AND D. SLEPČEV, A variational approach to the consistency of spectral clustering, Applied and Computational Harmonic Analysis, (2016).
- [22] N. GARCÍA TRILLOS AND D. SLEPČEV, On the rate of convergence of empirical measures in
   ∞-transportation distance, Canadian Journal of Mathematics, 67 (2015), pp. 1358–1383.
- [23] N. GARCÍA TRILLOS AND D. SLEPČEV, Continuum limit of total variation on point clouds,
   Archive for Rational Mechanics and Analysis, 220 (2016), pp. 193–241.
- [24] J. E. GILBERT, Interpolation between weighted L<sup>p</sup>-spaces, Ark. Mat., 10 (1972), pp. 235–249,
   doi:10.1007/BF02384812, http://dx.doi.org/10.1007/BF02384812.
- [25] D. GRIESER, Uniform bounds for eigenfunctions of the Laplacian on manifolds with bound ary, Comm. Partial Differential Equations, 27 (2002), pp. 1283–1299, doi:10.1081/PDE 120005839, https://doi.org/10.1081/PDE-120005839.
- <sup>753</sup> [26] P. GRISVARD, Elliptic problems in nonsmooth domains, SIAM, 2011.
- [27] L. HÖRMANDER, The spectral function of an elliptic operator, Acta Math, 121 (1968), pp. 193–
   218.
- [28] M. A. IGLESIAS, Y. LU, AND A. M. STUART, A Bayesian level set method for geometric inverse
   problems, Interfaces and Free Boundary Problems, (2015).
- [29] G. LEONI, A first course in Sobolev spaces, vol. 181 of Graduate Studies in Mathematics,
   American Mathematical Society, Providence, RI, second ed., 2017.
- [30] S. Z. LI, Markov random field modeling in computer vision, Springer Science & Business Media,
   2012.
- [31] A. MADRY, Fast approximation algorithms for cut-based problems in undirected graphs, in
   Foundations of Computer Science (FOCS), 2010 51st Annual IEEE Symposium on, IEEE,
   2010, pp. 245–254.
- [32] B. NADLER, N. SREBRO, AND X. ZHOU, Semi-supervised learning with the graph Laplacian:
   The limit of infinite unlabelled data, in Advances in neural information processing systems,
   2009, pp. 1330–1338.
- [33] R. NEAL, Regression and classification using Gaussian process priors, Bayesian Statistics, 6
   (1998), p. 475. Available at http://www.cs.toronto. edu/ radford/valencia.abstract.html.
- [34] A. Y. NG, M. I. JORDAN, AND Y. WEISS, On spectral clustering: Analysis and an algorithm,
   in Advances in neural information processing systems, 2002, pp. 849–856.
- [35] J. PEETRE, On an interpolation theorem of Foiaş and Lions, Acta Sci. Math. (Szeged), 25 (1964), pp. 255–261.
- [36] J. SHI AND J. MALIK, Normalized cuts and image segmentation, IEEE Transactions on pattern analysis and machine intelligence, 22 (2000), pp. 888–905.
- [37] Z. SHI, S. OSHER, AND W. ZHU, Weighted nonlocal Laplacian on interpolation from sparse data, Journal of Scientific Computing, 73 (2017), pp. 1164–1177.
- [38] D. SLEPČEV AND M. THORPE, Analysis of p-Laplacian regularization in semi-supervised learning, arXiv preprint arXiv:1707.06213, (2017).
- [39] C. D. SOGGE AND S. ZELDITCH, Riemannian manifolds with maximal eigenfunction growth, Duke Math. J., 114 (2002), pp. 387–437, https://doi.org/10.1215/S0012-7094-02-11431-8.

- [40] A. SZLAM AND X. BRESSON, Total variation and Cheeger cuts, in Proceedings of the 27th 782 International Conference on Machine Learning, 2010, pp. 1039–1046. 783
- [41] M. THORPE AND A. M. JOHANSEN, Convergence and rates for fixed-interval multiple-track 784 smoothing using k-means type optimization, Electronic Journal of Statistics, 10 (2016), 785 pp. 3693-3722. 786
- [42] M. THORPE AND F. THEIL, Asymptotic analysis of the Ginzburg-Landau functional on point 787 clouds, to appear in the Proceedings of the Royal Society of Edinburgh Section A: Mathe-788 matics, arXiv preprint arXiv:1604.04930, (2017). 789
- [43] M. THORPE, F. THEIL, A. M. JOHANSEN, AND N. CADE, Convergence of the k-means mini-790 791 mization problem using  $\Gamma$ -convergence, SIAM Journal on Applied Mathematics, 75 (2015), pp. 2444-2474. 792
- [44] Y. VAN GENNIP AND A. L. BERTOZZI,  $\Gamma$ -convergence of graph Ginzburg-Landau functionals, 793 Advances in Differential Equations, 17 (2012), pp. 1115–1180. 794
- [45] U. VON LUXBURG, A tutorial on spectral clustering, Statistics and computing, 17 (2007), 795 pp. 395-416. 796
- [46] U. VON LUXBURG, M. BELKIN, AND O. BOUSQUET, Consistency of spectral clustering, The 797 Annals of Statistics, (2008), pp. 555–586. 798
- [47]G. WAHBA, Spline models for observational data, SIAM, 1990. 799
- C. K. WILLIAMS AND C. E. RASMUSSEN, Gaussian processes for regression, in Advances in [48]800 neural information processing systems, 1996, pp. 514-520. 801
- [49] D. ZHOU, O. BOUSQUET, T. N. LAL, J. WESTON, AND B. SCHÖLKOPF, Learning with local and 802 global consistency, in Advances in neural information processing systems, 2004, pp. 321-803 328.804
- [50] X. ZHOU AND M. BELKIN, Semi-supervised learning by higher order regularization., in AIS-805 TATS, 2011, pp. 892–900. 806
- [51] X. ZHU, Semi-supervised learning literature survey, tech. report, Computer Science, University 807 of Wisconsin-Madison, 2005. 808
- [52] X. ZHU, Semi-supervised learning with graphs, PhD thesis, Carnegie Mellon University, lan-809 guage technologies institute, school of computer science, 2005. 810
- [53] X. ZHU, Z. GHAHRAMANI, AND J. LAFFERTY, Semi-supervised learning using Gaussian fields 811 and harmonic functions, in Proceedings of the 20th International Conference on Machine 812 Learning, vol. 3, 2003, pp. 912–919. 813
- [54] X. ZHU, J. D. LAFFERTY, AND Z. GHAHRAMANI, Semi-supervised learning: From Gaussian 814 fields to Gaussian processes, tech. report, CMU Tech Report:CMU-CS-03-175, 2003. 815

### 7. Appendix. 816

**7.1.** Function Spaces. Here we establish the equivalence between the spectrally 817 defined Sobolev spaces,  $\mathcal{H}^{s}(\Omega)$  and the standard Sobolev spaces. 818

We denote by 819

$$H_N^2(\Omega) = \left\{ u \in H^2(\Omega) : \frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega \right\}$$

the domain of  $\mathcal{L}$ . Analogously we denote by  $H^{2m}_N(\Omega)$  the domain of  $\mathcal{L}^m$ , that is 820

$$H_N^{2m}(\Omega) = \left\{ u \in H^{2m}(\Omega) : \frac{\partial \mathcal{L}^r u}{\partial n} = 0 \text{ for all } 0 \le r \le m - 1 \text{ on } \partial \Omega \right\}$$

821

Finally we let  $H_N^{2m+1}(\Omega) = H^{2m+1}(\Omega) \cap H_N^{2m}(\Omega)$ . For  $m \ge 0$  and  $u, v \in H_N^{2m+1}(\Omega)$  let  $\langle u, v \rangle_{2m+1,\mu} = \int_{\Omega} \nabla \mathcal{L}^m u \cdot \nabla \mathcal{L}^m v \rho^2 dx$  and for  $u, v \in H_N^{2m}(\Omega)$  let  $\langle u, v \rangle_{2m,\mu} = \int_{\Omega} (\mathcal{L}^m u) (\mathcal{L}^m v) \rho \, dx$ . We note that on the  $L^2_{\mu}$  orthogonal 822 823 complement of the constant function 1,  $\langle \cdot, \cdot \rangle_{2m+1,\mu}$  defines an inner product, which 824 due to Poincaré inequality is equivalent to the standard inner product on  $H^{2m+1}(\Omega)$ . 825 We also note that  $\langle \varphi_k, \varphi_k \rangle_{2m+1,\mu} = \lambda_k^{2m+1}$ , where we recall that  $\varphi_k$  is unit eigenvector 826 of  $\mathcal{L}$  corresponding to  $\lambda_k$ . 827

LEMMA 16. Under Assumptions 2 - 3, for any integer  $s \ge 0$ 828

$$H_N^s(\Omega) = \mathcal{H}^s(\Omega)$$
27

and the associated inner products  $\langle \cdot, \cdot \rangle_{s,\mu}$  and  $\langle \! \langle \cdot, \cdot \rangle \! \rangle_{s,\mu}$  are equivalent on the  $L^2_{\mu}$ 829 orthogonal complement of the constant function. 830

*Proof.* For s = 0,  $H_N^0 = L^2$  by definition and  $\mathcal{H}^0 = L^2$  by the fact that  $\{\varphi_k : k = 0\}$ 831  $1, \ldots$  is an orthonormal basis. 832

To show the claim for s = 1, we recall that  $\int \nabla \varphi_k \cdot \nabla \varphi_i \rho^2 dx = \int \varphi_k \mathcal{L} \varphi_i \rho dx =$ 833  $\lambda_k \delta_k^j$ . Therefore  $\left\{\frac{\varphi_k}{\sqrt{\lambda_k}}: k \ge 1\right\}$  is an orthonormal basis of the orthogonal complement 834 of the constant function,  $1^{\perp}$ , in  $H_N^1$  with respect to inner product  $(u, v) = \int \nabla_u \cdot$ 835  $\nabla v \rho^2 dx$  which is equivalent to the standard inner product of  $H_N^1$  on  $1^{\perp}$ . Since an 836 expansion in the basis  $\{\varphi_k\}_k$  is unique, this implies that for any  $u \in H^1_N = H^1$  the 837 series  $\sum_k a_k \varphi_k$  converges in  $H^1$  to u. Consequently if  $u \in H^1_N$  then  $\infty > \int |\nabla u|^2 \rho^2 dx =$ 838  $\int |\sum_k a_k \nabla \varphi_k|^2 \rho^2 dx = \sum_k a_k^2 \lambda_k \text{ which implies that } u \in \mathcal{H}^1. \text{ So } H^1_N \subseteq \mathcal{H}^1.$ 839

On the other hand, if  $u \in \mathcal{H}^1$  then  $u = \sum_k a_k \varphi_k$  with  $\sum_k \lambda_k a_k^2 < \infty$ . Therefore  $u = \bar{u} + \sum_{k=2}^{\infty} a_k \sqrt{\lambda_k} \frac{\varphi_k}{\sqrt{\lambda_k}}$ , where  $\bar{u}$  is the average of u. Since  $\frac{\varphi_k}{\sqrt{\lambda_k}}$  are orthonormal in 840 841 scaler product with topology equivalent to  $H^1$ , the series converges in  $H^1$ . Therefore 842  $u \in H^1 = H^1_N.$ 843

Assume now that the claim holds for all integers less than s. We split the proof 844 of the induction step into two cases: 845

Case 1° Consider s even; that is s = 2m for some integer m > 0. 846

Assume  $u \in H_N^{2m}$ . Then  $\nabla \mathcal{L}^r u \cdot \vec{n} = 0$  on  $\partial \Omega$  for all r < m. By the induction 847 hypothesis  $\sum_k \lambda_k^{2m-1} a_k^2 < \infty$ . Since  $\mathcal{L}$  is a continuous operator from  $\mathcal{H}^2$  to  $L^2$  one obtains by induction that  $\mathcal{L}^{m-1} u = \sum_k a_k \mathcal{L}^{m-1} \varphi_k = \sum a_k \lambda_k^{m-1} \varphi_k$ . Let  $v = \mathcal{L}^{m-1} u$ . By 848 849 assumption  $v \in H_N^2$ . By above  $v = \sum_k a_k \lambda_k^{m-1} \varphi_k$ . 850

Since  $\varphi_k$  is solution of  $\mathcal{L}\varphi_k = \lambda_k \varphi_k$ 851

$$(\mathcal{L}\varphi_k, v)_{\mu} = \langle \lambda_k \varphi_k, v \rangle_{\mu}$$

Using that  $v \in H^2$ ,  $\nabla v \cdot \vec{n} = 0$  on  $\partial \Omega$  and integration by parts we obtain 852

(

$$\langle \varphi_k, \mathcal{L}v \rangle_{\mu} = \langle \lambda_k \varphi_k, \sum_j a_j \lambda_j^{m-1} \varphi_j \rangle_{\mu} = \lambda_k^m a_k$$

Given that  $\mathcal{L}v$  is an  $L^2_{\mu}$  function, we conclude that  $\mathcal{L}v = \sum_k \lambda_k^m a_k \varphi_k$ . Therefore 853  $\sum_{k} \lambda_k^{2m} a_k^2 < \infty$  and hence  $u \in \mathcal{H}^{2m}$ . 854

To show the opposite inclusion, consider  $u \in \mathcal{H}^{2m}$ . Then  $u = \sum_k a_k \varphi_k$  and  $\sum_{k} \lambda_k^{2m} a_k^2 < \infty.$  By induction step we know that  $u \in H_N^{2m-2}$  and thus  $v = \mathcal{L}^{m-1} u \in L^2.$ We conclude as before that  $v = \sum_k \lambda_k^{m-1} a_k \varphi_k$ . Let  $b_k = \lambda_k^{m-1} a_k$ . Assumptions on uimply  $\sum_k \lambda_k^2 b_k^2 < \infty$ . Arguing as above in the case s = 1 we conclude that the series converges in  $H^1$  and that  $\nabla v = \sum_k b_k \nabla \varphi_k$ . Combining this with the fact that  $\mathcal{L}\varphi_k = \lambda_k \varphi_k$  in  $\Omega$  for all k implies that v is a weak solution of

$$\mathcal{L}v = \sum_{k} \lambda_k b_k \varphi_k \quad \text{ in } \Omega,$$
$$\frac{\partial v}{\partial n} = 0 \quad \text{ on } \partial \Omega.$$

Since RHS of the equation is in  $L^2$  and  $\partial \Omega$  is  $C^{1,1}$ , by elliptic regularity [26],  $v \in H^2$  and 855

 $\|v\|_{H^2}^2 \leq C(\Omega, \rho) \sum_k b_k^2 \lambda_k^2$ . Furthermore v satisfies the Neumann boundary condition and thus  $v \in H_N^2$ . 856

857

Case 2° Consider s odd; that is s = 2m + 1 for some integer m > 0. Assume  $u \in \overline{H_N^{2m+1}}$ . Let  $v = \mathcal{L}^m u$ . Then  $v \in H^1$ . The result now follows analogously to the 859

case s = 1. If  $u \in \mathcal{H}^{2m+1}$  then,  $u = \sum_k a_k \varphi_k$  with  $\sum_k \lambda_k^{2m+1} a_k^2 < \infty$ . By induction hypothesis,  $v = \mathcal{L}^{m-1} u \in H_N^1$  and  $v = \sum_k b_k \varphi_k$  where  $b_k = \lambda^{m-1} a_k$ . Thus  $\sum_k \lambda_k b_k^2 < \infty$ and the argument proceeds as in the case s = 1.

Proving the equivalence of inner products is straightforward.

We now present the proof of Lemma 3.

Proof of Lemma 3. If s is integer the claim follows form Lemma 16 and Sobolev 865 embedding theorem. Assume  $s = m + \theta$  for some  $\theta \in (0, 1)$ . Since  $\Omega$  is Lipschitz, 866 by extension theorem of Stein (Leoni [29] 2nd edition, Theorem 13.17) there is a 867 bounded linear extension mapping  $E_m: H^m(\Omega) \to H^m(\mathbb{R}^d)$  such that  $E_m(f)|_{\Omega} = f$ . 868 From the construction (see remark 13.9 in [29]) it follows that  $E_m$  and  $E_{m+1}$  agree 869 on smooth functions and thus  $E_{m+1} = E_m|_{H^m(\Omega)}$ . Therefore, by Theorem 16.12 in 870 Leoni's book (or Lemma 3.7 of Abels [1])  $E_m$  provides a bounded mapping from the 871 interpolation space  $[H^m(\Omega), H^{m+1}(\Omega)]_{\theta,2} \to [H^m(\mathbb{R}^d), H^{m+1}(\mathbb{R}^d)]_{\theta,2}$ . As discussed above the statement of Lemma 3  $\mathcal{H}^{m+\theta}(\Omega) = [\mathcal{H}^m(\Omega), \mathcal{H}^{m+1}(\Omega)]_{\theta,2}$ . By Lemma 872 873 16,  $[\mathcal{H}^m(\Omega), \mathcal{H}^{m+1}(\Omega)]_{\theta,2}$  embeds into  $[H^m(\Omega), H^{m+1}(\Omega)]_{\theta,2}$ . Furthermore, we use 874 that, see Abels [1] Corollary 4.15,  $[H^m(\mathbb{R}^d), H^{m+1}(\mathbb{R}^d)]_{\theta,2} = H^{m+\theta}(\mathbb{R}^d)$ . Combining 875 these facts yields the existence of an bounded, linear, extension mapping  $\mathcal{H}^{m+\theta}(\Omega) \rightarrow$ 876  $H^{m+\theta}(\mathbb{R}^d)$ . The results (i) and (ii) follows by the Sobolev embedding theorem. 877

**7.2.** Passage from Discrete to Continuum. There are two key tools we use to pass from the discrete to continuum limit. The first is  $\Gamma$ -convergence.  $\Gamma$ convergence was introduced in the 1970's by De Giorgi as a tool for studying sequences of variational problems. More recently this methodology has been applied to study the large data limits of variational problems that arise from statistical inference, e.g. [21, 23, 41, 42, 43]. Accessible introductions to  $\Gamma$ -convergence can be found in [10, 16]

The  $\Gamma$ -convergence methodology provides a notion of convergence of functionals 885 that captures the behaviour of minimizers. In particular the minimizers converge 886 along a subsequence to a minimizer of the limiting functional. In our setting, the 887 objects of interest are functions on discrete domains and hence it is not immediate 888 how one should define convergence. This brings us to our second key tool. Recently 889 a suitable topology has been identified to characterize the convergence of discrete to 890 continuum using an optimal transport framework [23]. The main idea is, given a 891 discrete function  $u_n: \Omega_n \to \mathbb{R}$  and a continuum function  $u: \Omega \to \mathbb{R}$ , to include the 892 measures with respect to which they are defined in the comparison. Namely, one can 893 think of the function  $u_n$  as belonging to the  $L^p$  space over the empirical measure 894  $\mu_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$  and u belonging to the  $L^p$  space over the measure  $\mu$ . One defines 895 a continuum function  $\tilde{u}_n : \Omega \to \mathbb{R}$  by  $\tilde{u}_n = u_n \circ T_n$  where  $T_n : \Omega_n \to \Omega$  is a measure 896 preserving map between  $\mu$  and  $\mu_n$ . One then compares  $u_n$  and  $\tilde{u}_n$  in the  $L^p$  distance, 897 and simultaneously compares  $T_n$  and identity. In other words one considers both the 898 difference in values and the how far the matched points are. We give a brief overview 899 of  $\Gamma$ -convergence and the  $TL^p$  space. 900

7.2.1. A Brief Introduction to Γ-Convergence. We present the definition of Γ-convergence in terms of an abstract topology. In the next section we will discuss what topology we will use in our results. For now, we simply point out that the space  $\mathcal{X}$  needs to be general enough to include functions defined with respect to different measures. DEFINITION 17. Given a topological space  $\mathcal{X}$ , we say that a sequence of functions  $F_n : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$   $\Gamma$ -converges to  $F_\infty : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ , and we write  $F_\infty = \Gamma - \lim_{n \to \infty} F_n$ , if the following two conditions hold:

• (the limit inequality) for any convergent sequence  $u_n \rightarrow u$  in  $\mathcal{X}$ 

$$\liminf_{n \to \infty} F_n(u_n) \ge F_\infty(u)$$

• (the limsup inequality) for every  $u \in \mathcal{X}$  there exists a sequence  $u_n$  in  $\mathcal{X}$  with  $u_n \to u$  and

$$\limsup_{n \to \infty} F_n(u_n) \le F_\infty(u)$$

In the above definition we also call any sequence  $\{u_n\}_{n=1,...}$  that satisfies the limsup inequality a recovery sequence. The justification of  $\Gamma$ -convergence as the natural setting to study sequences of variational problems is given by the next proposition. The proof can be found in, for example, [10].

PROPOSITION 18. Let  $F_n, F_\infty : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ . Assume that  $F_\infty$  is the  $\Gamma$ -limit of  $F_n$  and the sequence of minimizers  $\{u_n\}_{n=1,\dots}$  of  $F_n$  is precompact. Then

$$\lim_{n \to \infty} \min_{\mathcal{X}} F_n = \lim_{n \to \infty} F_n(u_n) = \min_{\mathcal{X}} F_\infty$$

and furthermore, any cluster point u of  $\{u_n\}_{n=1,\ldots}$  is a minimizer of  $F_{\infty}$ .

<sup>919</sup> Note that  $\Gamma$ -  $\lim_{n\to\infty} F_n = F_\infty$  and  $\Gamma$ -  $\lim_{n\to\infty} G_n = G_\infty$  does not imply  $F_n + G_n \Gamma$ -<sup>920</sup> converges to  $G_\infty + F_\infty$ . Hence, in order to build optimization problems by considering <sup>921</sup> individual terms it is not enough, in general, to know that each term  $\Gamma$ -converges. In <sup>922</sup> particular, we consider using the quadratic form  $J_n^{(\alpha,\tau)}$  as a prior and adding fidelity <sup>923</sup> terms, e.g.

$$\mathsf{J}^{(n)}(u) = J_n^{(\alpha,\tau)}(u) + \Phi^{(n)}(u).$$

We show that, with probability one,  $\Gamma - \lim_{n \to \infty} J_n^{(\alpha,\tau)} = J_{\infty}^{(\alpha,\tau)}$ . In order to show that  $J^{(n)}$   $\Gamma$ -converges it suffices to show that  $\Phi^{(n)}$  converges along any sequence  $(\mu_n, u_n)$  along which  $J_n^{(\alpha,\tau)}(u_n)$  is finite. This is similar to the notion of continuous convergence, which is typically used [16, Proposition 6.20]. However we note that  $\Phi^{(n)}$  does not converge continuously since as a functional on  $TL^p(\Omega)$  it takes the value infinity whenever the measure considered is not  $\mu_n$ .

7.2.2. The  $TL^p$  Space. In this section we give an overview of the topology that was introduced in [23] to compare sequences of functions on graphs. We motivate the topology in the setting considered in this paper. Recall that  $\mu \in \mathcal{P}(\Omega)$  has density  $\rho$ and that  $\mu_n$  is the empirical measure. Given  $u_n : \Omega_n \to \mathbb{R}$  and  $u : \Omega \to \mathbb{R}$  the idea is to consider pairs  $(\mu, u)$  and  $(\mu_n, u_n)$  and compare them as such. We define the metric as follows.

DEFINITION 19. Given a bounded open set  $\Omega$ , the space  $TL^{p}(\Omega)$  is the space of pairs  $(\mu, f)$  such that  $\mu$  is a probability measure supported on  $\Omega$  and  $f \in L^{p}(\mu)$ . The metric on  $TL^{p}$  is defined by

$$d_{TL^{p}}((f,\mu),(g,\nu)) = \inf_{\pi \in \Pi(\mu,\nu)} \left( \int_{\Omega \times \Omega} |x-y|^{p} + |f(x) - g(y)|^{p} d\pi(x,y) \right)^{\frac{1}{p}}.$$

Above  $\Pi(\mu, \nu)$  is the set of transportation plans (i.e. couplings) between  $\mu$  and  $\nu$ ; that is the set of probability measures on  $\Omega \times \Omega$  whose first marginal is  $\mu$  and second marginal in  $\nu$ . For a proof that  $d_{TL^p}$  is a metric on  $TL^p$  see [23, Remark 3.4].

To connect the  $TL^p$  metric defined above with the ideas discussed previously we make several observations. The first is that when  $\mu$  has a continuous density then one can consider transport maps  $T: \Omega \to \Omega_n$  that satisfy  $T_{\#}\mu = \mu_n$  instead of transport plans  $\pi \in \Pi(\mu, \nu)$ . Hence, one can show that

$$d_{TL^{p}}((f,\mu),(g,\nu)) = \inf_{T:T_{\#}\mu=\nu} \left( \|\mathrm{Id} - T\|_{L^{p}(\mu)}^{p} + \|f - g \circ T\|_{L^{p}(\mu)}^{p} \right)^{\frac{1}{p}}$$

In the setting when we compare  $(\mu, u)$  and  $(\mu_n, u_n)$  the second term is nothing but  $\|u - \tilde{u}_n\|_{L^p(\mu)}^p$ , where  $\tilde{u}_n = u_n \circ T_n$  and  $T_n : \Omega \to \Omega_n$  is a transport map.

We note that for a sequence  $(\mu_n, u_n)$  to  $TL^p$  converge to  $(\mu, u)$  it is necessary 949 that  $\|\mathrm{Id} - T\|_{L^{p}(\mu)}$  converges to zero, in other words it is necessary that the measures 950  $\mu_n$  converge to  $\mu$  in *p*-optimal transportation distance. We recall that since  $\Omega$  is 951 bounded this is equivalent to weak convergence of  $\mu_n$  to  $\mu$ . Assuming this to be the 952 case, we call any sequence of transportation maps  $T_n$  satisfying  $(T_n)_{\#}\mu = \mu_n$  and 953  $\|\operatorname{Id} - T_n\|_{L^p(\mu)} \to 0$  a stagnating sequence. One can then show (see [23, Proposition 954 3.12) that convergence in  $TL^p$  is equivalent to weak<sup>\*</sup> convergence of measures  $\mu_n$ 955 to  $\mu$  and convergence  $\|u - u_n \circ T_n\|_{L^p(\mu)} \to 0$  for arbitrary sequence of stagnating 956 transportation maps. Furthermore if convergence  $||u - u_n \circ T_n||_{L^p(\mu)} \to 0$  holds for a 957 sequence of stagnating transportation maps it holds for every sequence of stagnating 958 transportation maps. 959

The intrinsic scaling of the graph Laplacian, i.e. the parameter  $\varepsilon_n$ , depends on how far one needs to move "mass" to couple  $\mu$  and  $\mu_n$ , that is on upper bounds on transportation distance between  $\mu$  and  $\mu_n$ . The following result can be found in [22], the lower bound in the scaling of  $\varepsilon = \varepsilon_n$  is so that there exists a stagnating sequence of transport maps with  $\frac{\|T_n - \text{Id}\|_{L^{\infty}}}{\varepsilon_n} \to 0$ .

PROPOSITION 20. Let  $\Omega \subset \mathbb{R}^d$  with  $d \geq 2$  be open, connected and bounded with Lipschitz boundary. Let  $\mu \in \mathcal{P}(\Omega)$  with density  $\rho$  which is bounded above and below by strictly positive constants. Let  $\Omega_n = \{x_i\}_{i=1}^n$  where  $x_i \stackrel{\text{iid}}{\sim} \mu$  and let  $\mu_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$  be the associated empirical measure. Then, there exists C > 0 such that, with probability one, there exists a sequence of transportation maps  $T_n : \Omega \to \Omega_n$  that pushes  $\mu$  onto  $\mu_n$  and such that

$$\limsup_{n \to \infty} \frac{\|T_n - \mathrm{Id}\|_{L^{\infty}(\Omega)}}{\delta_n} \le C$$

971 where

$$\delta_n = \begin{cases} \frac{(\log n)^{\frac{3}{4}}}{\sqrt{n}} & \text{if } d = 2\\ \left(\frac{\log n}{n}\right)^{\frac{1}{d}} & \text{if } d \ge 3. \end{cases}$$

**7.3. Estimates on Eigenvalues of the Graph Laplacian.** The following lemma is nonasymptotic and holds for all n. However we will use it in the asymptotic regime and note that our assumptions on  $\varepsilon$ , (5), and results of Proposition 20 ensure that the assumptions of the lemma are satisfied.

LEMMA 21. Consider the operator  $A^{(n)}$  defined in (1) for  $\alpha = 1$ . Assume that  $d_{\text{OT}^{\infty}}(\mu_n,\mu) < \varepsilon$ . Then the spectral radius  $\lambda_{max}$  of  $A^{(n)}$  is bounded by  $C\frac{1}{\varepsilon^2} + \tau^2$  where C > 0 is independent of n and  $\varepsilon$ .

Let R > 0 be such that  $\eta(3R) > 0$ . Assume that  $d_{OT^{\infty}}(\mu_n, \mu) < R\varepsilon$ . Then there exists c > 0, independent of n and  $\varepsilon$ , such that  $\lambda_{max} > c\frac{1}{\varepsilon^2} + \tau^2$ .

*Proof.* Let  $\overline{\eta}(x) = \eta((|x|-1)_+)$ . Note that  $\overline{\eta} \ge \eta$  and that since  $\eta$  is decreasing 981 and integrable  $\int_{\mathbb{R}^d} \overline{\eta}(x) dx < \infty$ . 982

Let T be the  $d_{OT^{\infty}}$  transport map from  $\mu$  to  $\mu_n$ . By assumption  $||T_n(x) - x|| \leq \varepsilon$ 983 a.e. By definition of  $A^{(n)}$ 984

$$\lambda_{max} = \sup_{\|u\|_{L^{2}_{\mu_{n}}}=1} \langle u, A^{(n)}u \rangle_{\mu_{n}} = \tau^{2} + \sup_{\|u\|_{L^{2}_{\mu_{n}}}=1} \langle u, s_{n}Lu \rangle_{\mu_{n}}$$

We estimate

$$\begin{split} \sup_{\|u\|_{L^{2}_{\mu_{n}}}=1} \langle u, s_{n}Lu \rangle_{\mu_{n}} &\leq \sup_{\frac{1}{n} \sum_{i=1}^{n} u_{i}^{2}=1} \frac{4}{\sigma_{\eta}} \sum_{i,j} \frac{1}{n^{2} \varepsilon^{d+2}} \eta \left( \frac{|x_{i} - x_{j}|}{\varepsilon} \right) (u_{i}^{2} + u_{j}^{2}) \\ &\leq \sup_{\frac{1}{n} \sum_{i=1}^{n} u_{i}^{2}=1} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{n^{2} \varepsilon^{d+2}} \eta \left( \frac{|x_{i} - x_{j}|}{\varepsilon} \right) u_{i}^{2} \\ &= \sup_{\frac{1}{n} \sum_{i=1}^{n} u_{i}^{2}=1} \frac{1}{n \varepsilon^{d+2}} \sum_{i=1}^{n} u_{i}^{2} \int_{\Omega} \eta \left( \frac{|x_{i} - T(x)|}{\varepsilon} \right) d\mu(x) \\ &\leq \sup_{\frac{1}{n} \sum_{i=1}^{n} u_{i}^{2}=1} \frac{1}{n \varepsilon^{d+2}} \sum_{i=1}^{n} u_{i}^{2} \int_{\Omega} \overline{\eta} \left( \frac{x_{i} - x}{\varepsilon} \right) d\mu(x) \\ &\leq \frac{1}{\varepsilon^{2}} \int_{\mathbb{R}^{d}} \overline{\eta}(z) dz \lesssim \frac{1}{\varepsilon^{2}}. \end{split}$$

Above  $\leq$  means  $\leq$  up to a factor independent of  $\varepsilon$  and n. 985

To prove the second claim of the lemma consider  $v = \sqrt{n}\delta_{x_i}$ , a singleton concentrated at an arbitrary  $x_i$ , that is  $v_i = \sqrt{n}$  and  $v_j = 0$  for all  $j \neq i$ . Then  $\|v\|_{L^2_{\mu_n}} = 1$ . Using that for a.e.  $x \in B(x_i, 2\varepsilon R), |x_i - T(x)| \leq 3\varepsilon R$  we estimate:

(25)  

$$\sup_{\|u\|_{L^{2}_{\mu_{n}}}=1} \langle u, s_{n}Lu \rangle_{\mu_{n}} \geq \langle v, s_{n}Lv \rangle_{\mu_{n}} \\
\gtrsim \sum_{j \neq i} \frac{n}{n^{2} \varepsilon^{d+2}} \eta \left( \frac{|x_{i} - x_{j}|}{\varepsilon} \right) \\
= \frac{1}{\varepsilon^{d+2}} \int_{\Omega \setminus T^{-1}(x_{i})} \eta \left( \frac{|x_{i} - T(x)|}{\varepsilon} \right) d\mu(x) \\
\geq \frac{1}{\varepsilon^{d+2}} \int_{B(x_{i}, 2\varepsilon R) \setminus B(x_{i}, \varepsilon R)} \eta(3R) d\mu(x) \gtrsim \frac{1}{\varepsilon^{2}}$$

which implies the claim. 986

An immediate corollary of the claim is the characterization of the energy of a 987 singleton. For any  $\alpha \ge 1$  and  $\tau \ge 0$ . 988

(26) 
$$J_n^{(\alpha,\tau)}(\delta_{x_i}) \sim \frac{1}{n} \left(\frac{1}{\varepsilon_n^2} + \tau^2\right)^{\alpha} \sim \frac{1}{n\varepsilon_n^{2\alpha}}.$$

The upper bound is immediate from the first part of the lemma, while the lower bound 989 follows from the second part of the lemma via Jensen's inequality. Namely,  $(\lambda_k^{(n)}, q_k^{(n)})$ be eigenpairs of L and let us expand  $\delta_{x_i}$  in the terms of  $q_k^{(n)}$ : i.e.  $\delta_{x_i} = \sum_{k=1}^n a_k q_k^{(n)}$ where  $\sum_k a_k^2 = \|\delta_{x_i}\|_{L^2_{\mu_n}}^2 = \frac{1}{n}$ . We know that  $\sum_k \lambda_k^{(n)} a_k^2 \gtrsim \frac{1}{n\varepsilon_n^2 s_n} \sim 1$ , from (25) (using 990 991 992 32

<sup>993</sup> the expansion (27) and noting that  $v = \sqrt{n}\delta_{x_i}$  in (25)). Hence

$$J_{n}^{(\alpha,\tau)}(\delta_{x_{i}}) = \frac{1}{2n} \sum_{k=1}^{n} \left( s_{n} \lambda_{k}^{(n)} + \tau^{2} \right)^{\alpha} n a_{k}^{2} \ge \frac{1}{2n} \left( n s_{n} \sum_{k=1}^{n} \lambda_{k}^{(n)} a_{k}^{2} + \tau^{2} \right)^{\alpha} \ge \frac{1}{2n} \left( \frac{1}{\varepsilon_{n}^{2}} + \tau^{2} \right)^{\alpha}.$$

994

7.4. The Limiting Quadratic Form. Here we prove Theorem 1. The key tool is to use spectral decomposition of the relevant quadratic forms, and to rely on the limiting properties of the eigenvalues and eigenvectors of L established in [21]. Let  $(q_k^{(n)}, \lambda_k^{(n)})$  be eigenpairs of L with eigenvalues  $\lambda_k$  ordered so that

$$0 = \lambda_1^{(n)} \le \lambda_2^{(n)} \le \lambda_3^{(n)} \le \dots \lambda_n^{(n)}$$

where  $\lambda_1^{(n)} < \lambda_2^{(n)}$  provided that the graph *G* is connected. We extend  $F : \mathbb{R} \to \mathbb{R}$  to a matrix-valued function *F* via  $F(L) = Q^{(n)}(\Lambda_F^{(n)})(Q^{(n)})^*$  where  $Q^{(n)}$  is the matrix with columns  $\{q_k^{(n)}\}_{k=1}^n$  and  $\Lambda_F^{(n)}$  is the diagonal matrix with entries  $\{F(\lambda_i^{(n)})\}_{i=1}^n$ . For constants  $\alpha \ge 1, \tau \ge 0$  and a scaling factor  $s_n$ , given by (6), we recall the definition of the precision matrix  $A^{(n)}$  is  $A^{(n)} = (s_n L + \tau^2 I)^{\alpha}$  and the fractional Sobolev energy  $J_n^{(\alpha,\tau)}$  is

$$J_n^{(\alpha,\tau)}: L^2_{\mu_n} \mapsto [0,+\infty), \qquad J_n^{(\alpha,\tau)}(u) = \frac{1}{2} \langle u, A^{(n)}u \rangle_{\mu_n}.$$

1005 Note that

(27) 
$$J_n^{(\alpha,\tau)}(u) = \frac{1}{2} \sum_{k=1}^n (s_n \lambda_k^{(n)} + \tau^2)^\alpha \langle u, q_k^{(n)} \rangle_{\mu_n}^2.$$

When showing  $\Gamma$ -convergence, all functionals are considered as functionals on the  $TL^p$ space. When evaluating  $J_n^{(\alpha,\tau)}$  at  $(\nu, u)$  we consider it infinite for any measure  $\nu$  other than  $\mu_n$ , and having the value  $J_n^{(\alpha,\tau)}(u)$  defined above if  $\nu = \mu_n$ .

We let  $(q_k, \lambda_k)$  for k = 1, 2, ... be eigenpairs of  $\mathcal{L}$  ordered so that

$$0 = \lambda_1 \le \lambda_2 \le \lambda_3 \le \dots$$

We extend  $F : \mathbb{R} \to \mathbb{R}$  to an operator valued function via the identity  $F(\mathcal{L}) = \sum_{k=1}^{\infty} F(\lambda_k) \langle u, q_k \rangle_{\mu} q_k$ . For constants  $\alpha \geq 1$  and  $\tau \geq 0$  we recall the definition of the precision operator  $\mathcal{A}$  as  $\mathcal{A} = (\mathcal{L} + \tau I)^{\alpha}$  and the continuum Sobolev energy  $J_{\infty}^{(\alpha,\tau)}$ as

$$J_{\infty}^{(\alpha,\tau)}: L^{2}_{\mu} \mapsto \mathbb{R} \cup \{+\infty\}, \qquad J_{\infty}^{(\alpha,\tau)}(u) = \frac{1}{2} \langle u, \mathcal{A}u \rangle_{\mu}.$$

<sup>1014</sup> Note that the Sobolev energy can be written

$$J_{\infty}^{(\alpha,\tau)}(u) = \frac{1}{2} \sum_{k=1}^{\infty} (\lambda_k + \tau^2)^{\alpha} \langle u, q_k \rangle_{\mu}^2.$$

Proof of Theorem 1. We prove the theorem in three parts. In the first part we prove the liminf inequality and in the second part the limsup inequality. The third part is devoted to the proof of the two compactness results.

The Liminf Inequality. Let  $u_n \to u$  in  $TL^p$ , we wish to show that 1018

$$\liminf_{n \to \infty} J_n^{(\alpha,\tau)}(u_n) \ge J_\infty^{(\alpha,\tau)}(u).$$

By [21, Theorem 1.2], if all eigenvalues of  $\mathcal{L}$  are simple, we have with probability one 1019 (where the set of probability one can be chosen independently of the sequence  $u_n$ 1020 and u) that  $s_n \lambda_k^{(n)} \to \lambda_k$  and  $q_k^{(n)}$  converge in  $TL^2$  to  $q_k$ . If there are eigenspaces of  $\mathcal{L}$  of dimension higher than one then  $q_k^{(n)}$  converge along a subsequence in  $TL^2$  to 1021 1022 eifenfunctions  $\tilde{q}_k$  corresponding to the same eigenvalue as  $q_k$ . In this case we replace  $q_k$ 1023 by  $\tilde{q}_k$ , which does not change any of the functionals considered. We note that while 1024 eigenvectors in the general case only converge along subsequences, the projections 1025 to the relevant spaces of eigenvectors converge along the whole sequence, see [21, 1026 statement 3. Theorem 1.2]. To prove the convergence of the functional one would 1027 need to use these projections, which makes the proof cumbersome. For that reason in 1028 the remainder of the proof we assume that all eigenvalues of  $\mathcal{L}$  are simple, in which 1029 case we can express the projections using the inner product with eigenfunctions. 1030

Since  $q_k^{(n)} \to q_k$  and  $u_n \to u$  in  $TL^2$  as  $n \to \infty$ ,  $\langle q_k^{(n)}, u_n \rangle_{\mu_n} \to \langle q, u \rangle_{\mu}$  as  $n \to \infty$ . First we assume that  $J_{\infty}^{(\alpha,\tau)}(u) < \infty$ . Let  $\delta > 0$  and choose K such that 1031 1032

$$\frac{1}{2}\sum_{k=1}^{K} (\lambda_k + \tau^2)^{\alpha} \langle u, q_k \rangle_{\mu}^2 \ge J_{\infty}^{(\alpha, \tau)}(u) - \delta.$$

Now,

$$\liminf_{n \to \infty} J_n^{(\alpha,\tau)}(u_n) \ge \liminf_{n \to \infty} \frac{1}{2} \sum_{k=1}^K (s_n \lambda_k^{(n)} + \tau^2)^\alpha \langle u_n, q_k^{(n)} \rangle_\mu^2$$
$$= \frac{1}{2} \sum_{k=1}^K (\lambda_k + \tau^2)^\alpha \langle u_n, q_k \rangle_\mu^2$$
$$\ge J_\infty^\alpha(u) - \delta.$$

Let  $\delta \to 0$  to complete the limit inequality for when  $J_{\infty}^{(\alpha,\tau)}(u) < \infty$ . If  $J_{\infty}^{(\alpha,\tau)}(u) = +\infty$  then choose any M > 0 and find K such that  $\frac{1}{2} \sum_{k=1}^{K} (\lambda_k + \tau^2)^{\alpha} (u_n, q_k)_{\mu}^2 \ge M$ , the same 1033 1034 argument as above implies that 1035

$$\liminf_{n \to \infty} J_n^{(\alpha, \tau)}(u_n) \ge M$$

and therefore  $\liminf_{n\to\infty} J_n^{(\alpha,\tau)}(u_n) = +\infty$ . 1036

The Limsup Inequality. As above, we assume for simplicity, that all eigenvalues 1037 of  $\mathcal{L}$  are simple. We remark that there are no essential difficulties to carry out the 1038 1039

proof in the general case. Let  $u \in L^2_{\mu}$  with  $J^{(\alpha,\tau)}_{\infty}(u) < \infty$  (the proof is trivial if  $J^{(\alpha,\tau)}_{\infty} = \infty$ ). Define  $u_n \in L^2_{\mu_n}$ 1040 by  $u_n = \sum_{k=1}^{K_n} \psi_k q_k^{(n)}$  where  $\psi_k = \langle u, q_k \rangle_{\mu}$ . Let  $T_n$  be the transport maps from  $\mu$  to  $\mu_n$ as in Proposition 20. Let  $a_k^n = \psi_k q_k^{(n)} \circ T_n$  and  $a_k = \psi_k q_k$ . By Lemma 24, there exists a sequence  $K_n \to \infty$  such that  $u_n$  converges to u in  $TL^2$  metric. 1041 1042 1043

We recall from the proof of the limit inequality that  $\langle q_k^{(n)}, u_n \rangle_{\mu_n} \to \langle q_k, u \rangle_{\mu}$  as 1044  $n \to \infty$ . Combining with the convergence of eigenvalues, [21, Theorem 1.2], implies 1045

$$(s_n\lambda_k^{(n)} + \tau^2)^{\alpha} \langle u_n, q_k^{(n)} \rangle_{\mu_n}^2 \to (\lambda_k + \tau^2)^{\alpha} \langle u, q_k \rangle_{\mu}^2$$
34

as  $n \to \infty$ . Taking  $a_k^n = (s_n \lambda_k^{(n)} + \tau^2)^{\alpha} \langle u_n, q_k^{(n)} \rangle_{\mu_n}^2$  and  $a_k = (\lambda_k + \tau^2)^{\alpha} \langle u, q_k \rangle_{\mu}^2$  and using Lemma 24 implies that there exists  $\tilde{K}_n \leq K_n$  converging to infinity such that  $\sum_{k=1}^{\tilde{K}_n} a_k^n \to \sum_{k=1}^{\infty} a_k$  as  $n \to \infty$ . Let  $\tilde{u}_n = \sum_{k=1}^{\tilde{K}_n} \psi_k q_k^{(n)}$ . Then  $\tilde{u}_n \to u$  in  $TL^2$ . Furthermore  $J_n^{(\alpha,\tau)}(\tilde{u}_n) = \sum_{k=1}^{\tilde{K}_n} a_k^n$  and  $J_{\infty}^{(\alpha,\tau)}(u) = \sum_{k=1}^{\infty} a_k$  which implies that  $J_n^{(\alpha,\tau)}(\tilde{u}_n) \to J_{\infty}^{(\alpha,\tau)}(u)$  as  $n \to \infty$ .

1051 Compactness. If  $\tau > 0$  and  $\sup_{n \in \mathbb{N}} J_n^{(\alpha, \tau)}(u_n) \le C$  then

$$\tau^{2\alpha} \|u_n\|_{L^2_{\mu_n}}^2 = \tau^{2\alpha} \sum_{k=1}^n \langle u_n, q_k^{(n)} \rangle_{\mu_n}^2 \le \sum_{k=1}^n (s_n \lambda_k^{(n)} + \tau^2)^\alpha \langle u_n, q_k^{(n)} \rangle_{\mu_n}^2 \le C.$$

Therefore  $||u_n||_{L^2_{\mu_n}}$  is bounded. Hence in statements 2 and 3 of the theorem we have that  $||u_n||_{L^2_{\mu_n}}$  and  $J_n^{(\alpha,\tau)}(u_n)$  are bounded. That is there exists C > 0 such that

(28) 
$$||u||^2_{L^2_{\mu_n}} = \sum_{k=1}^n \langle u_n, q_k^{(n)} \rangle_{\mu_n} \le C \text{ and } s_n^{\alpha} \sum_{k=1}^n (\lambda_k^{(n)})^{\alpha} \langle u_n, q_k^{(n)} \rangle_{\mu_n}^2 \le C.$$

We will show there exists  $u \in L^2_{\mu}$  and a subsequence  $n_m$  such that  $u_{n_m}$  converges to uin  $TL^2$ .

Let  $\psi_k^n = \langle u_n, q_k^{(n)} \rangle_{\mu_n}$  for all  $k \leq n$ . Due to (28)  $|\psi_k^n|$  are uniformly bounded. Therefore, by a diagonal procedure, there exists a increasing sequence  $n_m \to \infty$  as  $m \to \infty$ such that for every k,  $\psi_k^{n_m}$  converges as  $m \to \infty$ . Let  $\psi_k = \lim_{m \to \infty} \psi_k^{n_m}$ . By Fatou's lemma,  $\sum_{k=1}^{\infty} |\psi_k|^2 \leq \liminf_{m \to \infty} \sum_{k=1}^{n_m} |\psi_k^{n_m}|^2 \leq C$ . Therefore  $u := \sum_{k=1}^{\infty} \psi_k q_k \in L^2_{\mu}$ . Using Lemma 24 and arguing as in the proof of the limsup inequality we obtain that there exists a sequence  $K_m$  increasing to infinity such that  $\sum_{k=1}^{K_m} \psi_k^{n_m} q_k^{(n_m)}$  converges to u in  $TL^2$  metric as  $m \to \infty$ . To show that  $u_{n_m}$  converges to u in  $TL^2$ , we now only need to show that  $||u_{n_m} - \sum_{k=1}^{K_m} \psi_k^{n_m} q_k^{(n_m)}||_{L^2_{\mu_{n_m}}}$  converges to zero. This follows from the fact that

$$\sum_{k=K_m+1}^{n_m} |\psi_k^{n_m}|^2 \le \frac{1}{\left(\lambda_{K_m}^{(n_m)}\right)^{\alpha}} \sum_{k=K_m+1}^{n_m} (\lambda_k^{(n_m)})^{\alpha} |\psi_k^{n_m}|^2 \le \frac{C}{\left(s_{n_m}\lambda_{K_m}^{(n_m)}\right)^{\alpha}}$$

using that the sequence of eigenvalues is nondecreasing. Now since  $s_{n_m}\lambda_{K_m}^{(n_m)} \geq s_{n_m}\lambda_{K}^{(n_m)} \rightarrow \lambda_K$  for all  $K_m \geq K$ , and  $\lim_{K\to\infty} \lambda_K = +\infty$  we have that  $s_{n_m}\lambda_{K_m}^{(n_m)} \rightarrow +\infty$ as  $m \rightarrow \infty$ , hence  $u_{n_m}$  converges to u in  $TL^2$ .

Remark 22. Note that when  $\alpha \ge 1$  the compactness property holds trivially from the compactness property for  $\alpha = 1$ , see [21, Theorem 1.4], as  $J_n^{(\alpha,\tau)}(u_n) \ge J_n^{(1,0)}(u_n)$ .

7.5. Variational Convergence of Probit in Labelling Model 1. To prove 1070 minimizers of the Probit model in Labelling Model 1 converge we apply Proposi-1071 tion 18. This requires us to show that  $J_p^{(n)}$   $\Gamma$ -converges to  $J_p^{(\infty)}$  and the compactness of sequences of minimizers. Recall that  $J_p^{(n)} = J_n^{(\alpha,\tau)} + \frac{1}{n} \Phi_p^{(n)}(\cdot;\gamma)$ . Hence Theorem 1 1072 107 establishes the  $\Gamma$ -convergence of the first term. We now show that  $\frac{1}{n}\Phi_{p}^{(n)}(u_{n};y_{n};\gamma) \rightarrow \Phi_{p,1}(u;y;\gamma)$  whenever  $(\mu_{n},u_{n}) \rightarrow (\mu,u)$  in the  $TL^{2}$  sense, which is enough to es-1074 1075 tablish  $\Gamma$ -convergence. Namely since, by definition,  $J_n^{(\alpha,\tau)}$  applied to an element 1076  $(\nu, v) \in TL^p(\Omega)$  is  $\infty$  if  $\nu \neq \mu_n$  it suffices to consider sequences of the form  $(\mu_n, u_n)$ 1077 to show the liminf inequality. The limsup inequality is also straightforward since the 1078 the recovery sequence for  $J_{\infty}^{(\alpha,\tau)}$  is also of the form  $(\mu_n, u_n)$ . 1079

LEMMA 23. Consider domain  $\Omega$  and measure  $\mu$  satisfying Assumptions 2–3. Let  $x_i \stackrel{\text{iid}}{\sim} \mu$  for i = 1, ..., n,  $\Omega_n = \{x_1, ..., x_n\}$  and  $\mu_n$  be the empirical measure of the sample. Let  $\Omega'$  be an open subset of  $\Omega$ ,  $\mu'_n = \mu_n \lfloor_{\Omega'}$  and  $\mu' = \mu \lfloor_{\Omega}$ . Let  $y_n \in L^{\infty}(\mu'_n)$  and  $y \in L^{\infty}(\mu')$  and let  $\hat{y}_n \in L^{\infty}(\mu_n)$  and  $\hat{y} \in L^{\infty}(\mu)$  be their extensions by zero. Assume

$$(\mu_n, \hat{y}_n) \to (\mu, \hat{y}) \quad in \ TL^{\infty} \ as \ n \to \infty.$$

Let  $\Phi_{\mathbf{p}}^{(n)}$  and  $\Phi_{\mathbf{p},1}$  be defined by (9) and (16) respectively, where  $Z' = \{j : x_j \in \Omega'\}$ and  $\gamma > 0$  (and where we explicitly include the dependence of  $y_n$  and y in  $\Phi_{\mathbf{p}}^{(n)}$  and  $\Phi_{\mathbf{p},1}$ ).

1087 Then, with probability one, if  $(\mu_n, u_n) \rightarrow (\mu, u)$  in  $TL^p$  then

$$\frac{1}{n}\Phi_{\mathbf{p}}^{(n)}(u_n;y_n;\gamma) \to \Phi_{\mathbf{p},1}(u;y;\gamma) \quad as \ n \to \infty$$

*Proof.* Let  $(\mu_n, u_n) \to (\mu, u)$  in  $TL^p$ . We first note that since  $\Psi(uy; \gamma) = \Psi\left(\frac{uy}{\gamma}; 1\right)$  and since multiplying all functions by a constant does not affect the  $TL^p$  convergence, it suffices to consider  $\gamma = 1$ . For brevity, we omit  $\gamma$  in the functionals that follow. We have that  $\hat{y}_n \circ T_n \to \hat{y}$  and  $u_n \circ T_n \to u$ . Recall that

$$\frac{1}{n} \Phi_{\mathbf{p}}^{(n)}(u_n; y_n) = \int_{T_n^{-1}(\Omega'_n)} \log \Psi(y_n(T_n(x))u_n(T_n(x))) \, \mathrm{d}\mu(x)$$
  
$$\Phi_{\mathbf{p},1}(u; y) = \int_{\Omega'} \log \Psi(y(x)u(x)) \, \mathrm{d}\mu(x),$$

where  $\Omega'_n = \{x_i : x_i \in \Omega', \text{ for } i = 1, ..., n\}$ . Recall also that symmetric difference of sets is denoted by  $A \triangle B = (A \smallsetminus B) \cup (B \smallsetminus A)$ . It follows that

(29) 
$$\left| \frac{1}{n} \Phi_{p}^{(n)}(u_{n}; y_{n}) - \Phi_{p,1}(u; y) \right| \leq \left| \int_{\Omega' \bigtriangleup T_{n}^{-1}(\Omega'_{n})} \log \Psi(\hat{y}(x)u(x)) d\mu(x) \right| + \left| \int_{T_{n}^{-1}(\Omega'_{n})} \log \left( \Psi(y_{n}(T_{n}(x))u_{n}(T_{n}(x)); \gamma) - \log \left( \hat{y}(x)u(x) \right) d\mu(x) \right| \right|$$

1088 Define

$$\partial_{\varepsilon_n} \Omega' = \{x : \operatorname{dist}(x, \partial \Omega') \le \varepsilon_n\}.$$

Then  $\Omega' riangleq T_n^{-1}(\Omega'_n) \subseteq \partial_{\varepsilon_n} \Omega'$ . Since  $\hat{y} \in L^{\infty}$  and  $u \in L^2_{\mu}$  then  $\hat{y}u \in L^2_{\mu}$  and so by Corollary 26 log  $\Psi(\hat{y}u) \in L^1$ . Hence, by the dominated convergence theorem

$$\left| \int_{\Omega' \triangle T_n^{-1}(\Omega'_n)} \log \Psi(\hat{y}(x)u(x)) \mathrm{d}\mu(x) \right| \le \int_{\partial_{\varepsilon_n} \Omega'} \left| \log \Psi(\hat{y}(x)u(x)) \right| \mathrm{d}\mu(x) \to 0.$$

We are left to show that the second term on the right hand side of (29) converges to 0. Let  $F(w, v) = |\log \Psi(w) - \log \Psi(v)|$ . Let  $M \ge 1$  and define the following sets

$$\mathcal{A}_{n,M} = \left\{ x \in T_n^{-1}(\Omega'_n) : \min\{\hat{y}(x)u(x), y_n(T_n(x))u_n(T_n(x))\} \ge -M \right\}$$
  
$$\mathcal{B}_{n,M} = \left\{ x \in T_n^{-1}(\Omega'_n) : \hat{y}(x)u(x) \ge y_n(T_n(x))u_n(T_n(x)) \le -M \right\}$$
  
$$\mathcal{C}_{n,M} = \left\{ x \in T_n^{-1}(\Omega'_n) : y_n(T_n(x))u_n(T_n(x)) \ge \hat{y}(x)u(x) \le -M \right\}.$$

The quantity we want to estimate satisfies

$$\left| \int_{T_n^{-1}(\Omega'_n)} \log \left( \Psi(y_n(T_n(x))u_n(T_n(x))) - \log \Psi(\hat{y}(x)u(x)) \, \mathrm{d}\mu(x) \right) \right| \\ \leq \int_{T_n^{-1}(\Omega'_n)} F(y_n(T_n(x))u_n(T_n(x)), \hat{y}(x)u(x)) \, \mathrm{d}\mu(x).$$

Since  $T_n^{-1}(\Omega'_n) = \mathcal{A}_{n,M} \cup \mathcal{B}_{n,M} \cup \mathcal{C}_{n,M}$  we proceed by estimating the integral over each of the sets, utilizing the bounds in Lemma 25.

$$\begin{aligned} \int_{\mathcal{A}_{n,M}} F(y_n(T_n(x))u_n(T_n(x)), \hat{y}(x)u(x)) \, \mathrm{d}\mu(x) \\ &\leq \frac{1}{\int_{-\infty}^{-M} e^{-\frac{t^2}{2}} \, \mathrm{d}t} \int_{\mathcal{A}_{n,M}} |y_n(T_n(x))u_n(T_n(x)) - \hat{y}(x)u(x)| \, \mathrm{d}\mu(x) \\ &\leq \frac{1}{\int_{-\infty}^{-M} e^{-\frac{t^2}{2}} \, \mathrm{d}t} \left( \|y_n\|_{L^2_{\mu_n}} \|u_n \circ T_n - u\|_{L^2_{\mu}} + \|u\|_{L^2_{\mu}} \|\hat{y}_n \circ T_n - \hat{y}\|_{L^2_{\mu}} \right) \end{aligned}$$

$$\begin{split} &\int_{\mathcal{B}_{n,M}} F(y_n(T_n(x))u_n(T_n(x)), \hat{y}(x)u(x)) \,\mathrm{d}\mu(x) \\ &\leq \int_{\mathcal{B}_{n,M}} 2|y_n(T_n(x))|^2 |u_n(T_n(x))|^2 \,\mathrm{d}\mu(x) + \frac{1}{M^2} \\ &\leq 2\|\hat{y}_n\|_{L^{\infty}_{\mu_n}}^2 \int_{\mathcal{B}_{n,M}} |u_n(T_n(x))|^2 \,\mathrm{d}\mu(x) + \frac{1}{M^2} \\ &\leq 4\|\hat{y}_n\|_{L^{\infty}_{\mu_n}}^2 \left( \|u_n \circ T_n - u\|_{L^2_{\mu}}^2 + \int_{\Omega} |u(x)|^2 \mathbb{I}_{|y_n(T_n(x))u_n(T_n(x))| \ge M} \,\mathrm{d}\mu(x) \right) + \frac{1}{M^2}. \end{split}$$

$$\begin{split} &\int_{\mathcal{C}_{n,M}} F(y_n(T_n(x))u_n(T_n(x)), \hat{y}(x)u(x)) \,\mathrm{d}\mu(x) \\ &\leq \int_{\mathcal{C}_{n,M}} 2|\hat{y}(x)|^2 |u(x)|^2 \,\mathrm{d}\mu(x) + \frac{1}{M^2} \\ &\leq 2\|\hat{y}\|_{L^\infty_{\mu}}^2 \int_{\Omega} |u(x)|^2 \mathbb{I}_{|y(x)u(x)| \geq M} \,\mathrm{d}\mu(x) + \frac{1}{M^2}. \end{split}$$

For every subsequence there exists a further subsequence such that  $(y_n \circ T_n)(u_n \circ T_n) \rightarrow yu$  pointwise a.e., hence by the dominated convergence theorem

$$\int_{\Omega} |u(x)|^2 \mathbb{I}_{|y_n(T_n(x))u_n(T_n(x))| \ge M} \,\mathrm{d}\mu(x) \to \int_{\Omega} |u(x)|^2 \mathbb{I}_{|y(x)u(x)| \ge M} \,\mathrm{d}\mu(x) \quad \text{as } n \to \infty.$$

Hence, for  $M \ge 1$  fixed we have

$$\begin{split} \limsup_{n \to \infty} \left| \int_{T_n^{-1}(\Omega'_n)} \log \left( \Psi(y_n(T_n(x))u_n(T_n(x));\gamma) - \log \left(\hat{y}(x)u(x);\gamma\right) \, \mathrm{d}\mu(x) \right| \\ & \leq \frac{2}{M^2} + 6 \|\hat{y}\|_{L^\infty_\mu} \int_{\Omega} |u(x)|^2 \mathbb{I}_{|\hat{y}(x)u(x)| \geq M} \, \mathrm{d}\mu(x). \end{split}$$

1095 Taking  $M \to \infty$  completes the proof.

<sup>1096</sup> The proof of Theorem 10 is now just a special case of the above lemma and an <sup>1097</sup> easy compactness result that follows from Theorem 1.

<sup>1098</sup> Proof of Theorem 10. The following statements all hold with probability one. Let

$$y(x) = \begin{cases} 1 & \text{if } x \in \Omega^+ \\ -1 & \text{if } x \in \Omega^-. \\ 37 \end{cases}$$

Since dist $(\Omega^+, \Omega^-) > 0$  there exists a minimal Lipschitz extension  $\hat{y} \in L^{\infty}$  of y to  $\Omega$ . Let  $y_n = y \lfloor_{\Omega_n}$  and  $\hat{y}_n = \hat{y} \lfloor_{\Omega_n}$ . Since

$$\begin{aligned} \|\hat{y}_n \circ T_n - \hat{y}\|_{L^{\infty}(\mu)} &= \mu \operatorname{ess\,sup}_{x \in \Omega} |\hat{y}_n(T_n(x)) - \hat{y}(x)| \\ &= \mu \operatorname{ess\,sup}_{x \in \Omega} |\hat{y}(T_n(x)) - \hat{y}(x)| \\ &\leq \operatorname{Lip}(\hat{y}) \|T_n - \operatorname{Id}\|_{L^{\infty}} \end{aligned}$$

we conclude that  $(\mu_n, \hat{y}_n) \to (\mu, \hat{y})$  in  $TL^{\infty}$ . Hence, by Lemma 23,  $\frac{1}{n} \Phi_p^{(n)}(u_n; \gamma) \to \Phi_{p,1}(u; \gamma)$  whenever  $(\mu_n, u_n) \to (\mu, u)$  in  $TL^p$ . Combining with Theorem 1 implies that  $\mathsf{J}_p^{(n)}$   $\Gamma$ -converges to  $\mathsf{J}_p^{(\infty)}$  via a straightforward argument. 1099 1100 1101

If  $\tau > 0$  then the compactness of minimizers follows from Theorem 1 using that 1102  $\sup_{n \in \mathbb{N}} \min_{v_n \in L^2_{\mu_n}} \mathsf{J}_{\mathrm{p}}^{(n)}(v_n) \leq \sup_{n \in \mathbb{N}} \mathsf{J}_{\mathrm{p}}^{(n)}(0) = \frac{1}{2}.$ 1103

When  $\tau = 0$  we consider the sequence  $w_n = v_n - \bar{v}_n$  where  $v_n$  is a minimizer of  $J_p^{(n)}$ 1104 and  $\bar{v}_n = (v_n, q_1)_{\mu_n} = \int_{\Omega} v_n(x) d\mu_n(x)$ . Then,  $J_n^{(\alpha,0)}(w_n) = J_n^{(\alpha,0)}(v_n)$  and 1105

$$\|w_n\|_{L^2_{\mu_n}}^2 = \|v_n - \bar{v}_n\|_{L^2_{\mu_n}}^2 = \sum_{k=2}^n \langle v_n, q_k \rangle_{\mu_n}^2 \le \frac{1}{(s_n \lambda_2^{(n)})^{\alpha}} J_n^{(\alpha,0)}(v_n).$$

As in the case  $\tau > 0$  the quadratic form is bounded, i.e.  $\sup_{n \in \mathbb{N}} \mathcal{J}_{p}^{(n)}(v_{n}) \leq \frac{1}{2}$ . Hence 1106  $J_n^{(\alpha,\tau)}(w_n) \leq \frac{1}{2}$  and  $||w_n||_{L^2_{\mu_n}}^2 \leq \frac{1}{\lambda_2^{\alpha}}$  for *n* large enough. By Theorem 1  $w_n$  is precompact 1107 in  $TL^2$ . Therefore  $\sup_{n \in \mathbb{N}} \|v_n\|_{L^2_{\mu_n}} \leq M + \sup_{n \in \mathbb{N}} |\bar{v}_n|$  for some M > 0. Since  $J_n^{(\alpha,\tau)}$  is insensitive to the addition of a constant, and  $-1 \leq y \leq 1$ , then for any minimiser  $v_n$ 1108 1109 one must have  $\bar{v}_n \in [-1,1]$ . Hence  $\sup_{n \in \mathbb{N}} \|v_n\|_{L^2_{\mu_n}} \leq M+1$  so by Theorem 1  $\{v_n\}$  is 1110 precompact in  $TL^2$ . 1111

Since the minimizers of  $J_p^{(\infty)}$  are unique (due to convexity, see Lemma 9), by 1112 Proposition 18 we have that the sequence of minimizers  $v_n$  of  $J_p^{(n)}$  converges to the 1113 minimizer of  $J_p^{(\infty)}$ . 1114

### 7.6. Variational Convergence of Probit in Labelling Model 2. 1115

Proof of Theorem 11. It suffices to show that  $J_{\rm p}^{(n)}$   $\Gamma$ -converges in  $TL^2$  to  $J_{\infty}^{(\alpha,\tau)}$ 1116 and that the sequence of minimizers  $v_n$  of  $J_p^{(n)}$  is precompact in  $TL^2$ . We note that 1117 the limit statement of the  $\Gamma$ -convergence follows immediately from statement 1. of 1118 Theorem 1. 1119

To complete the proof of  $\Gamma$ -convergence it suffices to construct a recovery sequence. 1120 The strategy is analogous to the one of the proof on Theorem 4.9 of [38]. Let  $v \in$ 1121  $\mathcal{H}^{\alpha}(\Omega)$ . Since  $J_n^{(\alpha,\tau)}$   $\Gamma$ -converges to  $J_{\infty}^{(\alpha,\tau)}$  by Theorem 1 there exists Let  $v^{(n)} \in L^2_{\mu_n}$ 1122 such that  $J_n^{(\alpha,\tau)}(v^{(n)}) \to J_{\infty}^{(\alpha,\tau)}(v)$  as  $n \to \infty$ . Consider the functions 1123

$$\tilde{v}^{(n)}(x_i) = \begin{cases} c_n y(x_i) & \text{if } i = 1, \dots, N. \\ v^{(n)}(x_i) & \text{if } i = N+1, \dots, n \end{cases}$$

where  $c_n \to \infty$  and  $\frac{c_n}{\varepsilon_n^{2\alpha}n} \to 0$  as  $n \to \infty$ . 1124

Note that condition (5) implies that when  $\alpha < \frac{d}{2}$  then (20) still holds. There-1125 fore (26) implies that  $J_n^{(\alpha,\tau)}(c_n\delta_{x_i}) \to 0$  as  $n \to \infty$ . Also note that since  $c_n \to \infty$ , 1126  $\Phi_{\rm p}^{(n)}(\tilde{v}^{(n)};\gamma) \to 0$  as  $n \to \infty$ . It is now straightforward to show, using the form of the 1127 38

<sup>1128</sup> functional, the estimate on the energy of a singleton and the fact that  $\varepsilon_n n^{\frac{1}{2\alpha}} \to \infty$  as <sup>1129</sup>  $n \to \infty$ , that  $\mathsf{J}_p^{(n)}(\tilde{v}^{(n)}) \to J_{\infty}^{(\alpha,\tau)}(v)$  as desired.

The precompactness of  $\{v_n\}_{n \in \mathbb{N}}$  follows from Theorem 1. Since 0 is the unique minimizer of  $J_{\infty}^{(\alpha,\tau)}$ , due to  $\tau > 0$ , the above results imply that  $v^{(n)}$  converge to 0.

## 1132 7.7. Small Noise Limits.

<sup>1133</sup> Proof of Theorem 14. First observe that since Assumptions 2–3 hold and  $\alpha > d/2$ , <sup>1134</sup> the measure  $\nu_0$ , and hence the measures  $\nu_{p,1}, \nu_{p,2}, \nu_1$ , are all well-defined measures on <sup>1135</sup>  $L^2(\Omega)$  by Theorem 4.

(i) For any continuous bounded function  $g: C(\Omega; \mathbb{R}) \to \mathbb{R}$  we have

$$\mathbb{E}^{\nu_{p,1}}g(u) = \frac{\mathbb{E}^{\nu_0}e^{-\Phi_{p,1}(u;\gamma)}g(u)}{\mathbb{E}^{\nu_0}e^{-\Phi_{p,1}(u;\gamma)}}, \quad \mathbb{E}^{\nu_1}g(u) = \frac{\mathbb{E}^{\nu_0}\mathbb{1}_{B_{\infty,1}}(u)g(u)}{\mathbb{E}^{\nu_0}\mathbb{1}_{B_{\infty,1}}(u)}.$$

For the first convergence it thus suffices to prove that, as  $\gamma \rightarrow 0$ ,

$$\mathbb{E}^{\nu_0} e^{-\Phi_{\mathrm{p},1}(u;\gamma)} g(u) \to \mathbb{E}^{\nu_0} \mathbb{1}_{B_{\infty,1}}(u) g(u)$$

for all continuous functions  $g: C(\Omega; \mathbb{R}) \to [-1, 1]$ . We first define the standard normal cumulative distribution function  $\varphi(z) = \Psi(z, 1)$ , and note that we may write

$$\Phi_{\mathbf{p},1}(u;\gamma) = -\int_{x\in\Omega'} \log\Big(\varphi(y(x)u(x)/\gamma)\Big) \mathrm{d}x \ge 0.$$

In what follows it will be helpful to recall the following standard Mills ratio bound: for all t > 0,

(30) 
$$\varphi(t) \ge 1 - \frac{e^{-t^2/2}}{t\sqrt{2\pi}}.$$

1139 Suppose first that  $u \in B_{\infty,1}$ , then  $y(x)u(x)/\gamma > 0$  for a.e.  $x \in \Omega'$ . The 1140 assumption that  $\overline{\Omega^+} \cap \overline{\Omega^-} = \emptyset$  ensures that y is continuous on  $\Omega' = \Omega^+ \cup \Omega^-$ . 1141 As u is also continuous on  $\Omega'$ , given any  $\varepsilon > 0$ , we may find  $\Omega'_{\varepsilon} \subseteq \Omega'$  such that 1142  $y(x)u(x)/\gamma > \varepsilon/\gamma$  for all  $x \in \Omega'_{\varepsilon}$ . Moreover, these sets may be chosen such 1143 that  $\operatorname{leb}(\Omega' \smallsetminus \Omega'_{\varepsilon}) \to 0$  as  $\varepsilon \to 0$ . Applying the bound (30), we see that for any 1144  $x \in \Omega'_{\varepsilon}$ ,

$$\varphi(y(x)u(x)/\gamma) \ge 1 - \gamma \frac{e^{-u(x)^2 y(x)^2/2\gamma^2}}{u(x)y(x)\sqrt{2\pi}} \ge 1 - \gamma \frac{e^{-\varepsilon^2/2\gamma^2}}{\varepsilon\sqrt{2\pi}}.$$

Additionally, for any  $x \in \Omega' \setminus \Omega'_{\varepsilon}$ , we have  $\varphi(y(x)u(x)/\gamma) \ge \varphi(0) = 1/2$ . We deduce that

$$\begin{split} \Phi_{\mathbf{p},1}(u;\gamma) &= -\int_{\Omega_{\varepsilon}'} \log(\varphi(y(x)u(x)/\gamma) \,\mathrm{d}\mu(x) - \int_{\Omega' \smallsetminus \Omega_{\varepsilon}'} \log(\varphi(y(x)u(x)/\gamma) \,\mathrm{d}\mu(x)) \\ &\leq -\log\left(1 - \gamma \frac{e^{-\varepsilon^2/2\gamma^2}}{\varepsilon\sqrt{2\pi}}\right) \cdot \rho^+ \cdot \operatorname{leb}(\Omega_{\varepsilon}') + \log(2) \cdot \rho^+ \cdot \operatorname{leb}(\Omega' \smallsetminus \Omega_{\varepsilon}'). \end{split}$$

1145 1146 1147 The right-hand term may be made arbitrarily small by choosing  $\varepsilon$  small enough. For any given  $\varepsilon > 0$ , the left-hand term tends to zero as  $\gamma \to 0$ , and so we deduce that  $\Phi_{p,1}(u;\gamma) \to 0$  and hence

$$e^{-\Phi_{\mathbf{p},1}(u;\gamma)}g(u) \to g(u) = \mathbb{1}_{B_{\infty,1}}(u)g(u).$$
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Now suppose that  $u \notin B_{\infty,1}$ , and assume first that there is a subset  $E \subseteq \Omega'$ with  $\operatorname{leb}(E) > 0$  and y(x)u(x) < 0 for all  $x \in E$ . Then similarly to above, there exists  $\varepsilon > 0$  and  $E_{\varepsilon} \subseteq E$  with  $\operatorname{leb}(E_{\varepsilon}) > 0$  such that  $y(x)u(x)/\gamma < -\varepsilon/\gamma$ for all  $x \in E_{\varepsilon}$ . Observing that  $\varphi(t) = 1 - \varphi(-t)$ , we may apply the bound (30) to deduce that, for any  $x \in E_{\varepsilon}$ ,

$$\varphi(y(x)u(x)/\gamma) \le -\gamma \frac{e^{-u(x)^2 y(x)^2/2\gamma^2}}{u(x)y(x)\sqrt{2\pi}} \le \frac{\gamma}{\varepsilon\sqrt{2\pi}}$$

We therefore deduce that

$$\Phi_{\mathbf{p},1}(u;\gamma) \ge \int_{E_{\varepsilon}} -\log(\varphi(y(x)u(x)/\gamma) \,\mathrm{d}\mu(x))$$
$$\ge -\log\left(\frac{\gamma}{\varepsilon\sqrt{2\pi}}\right) \cdot \rho^{-} \cdot \operatorname{leb}(E_{\varepsilon}) \to \infty$$

from which we see that

$$e^{-\Phi_{p,1}(u;\gamma)}g(u) \to 0 = \mathbb{1}_{B_{\infty,1}}(u)g(u)$$

Assume now that  $y(x)u(x) \ge 0$  for a.e.  $x \in \Omega'$ . Since  $u \notin B_{\infty,1}$  there is a subset  $\Omega'' \subseteq \Omega'$  such that y(x)u(x) = 0 for all  $x \in \Omega''$ , y(x)u(x) > 0 a.e.  $x \in \Omega' \setminus \Omega''$ , and  $leb(\Omega'') > 0$ . We then have

$$\begin{split} \Phi_{\mathbf{p},1}(u;\gamma) &= -\int_{\Omega''} \log(\varphi(0)) \,\mathrm{d}\mu(x) - \int_{\Omega' \smallsetminus \Omega''} \log(\varphi(y(x)u(x)/\gamma) \,\mathrm{d}\mu(x) \\ &= \log(2)\mu(\Omega'') - \int_{\Omega' \smallsetminus \Omega''} \log(\varphi(y(x)u(x)/\gamma) \,\mathrm{d}\mu(x) \\ &\to \log(2)\mu(\Omega''). \end{split}$$

We hence have  $e^{-\Phi_{p}(u;y,\gamma)}g(u) \neq 0 = \mathbb{1}_{B_{\infty,1}}(u)g(u)$ . However, the event

$$D := \{ u \in C(\Omega; \mathbb{R}) \mid \text{There exists } \Omega'' \subseteq \Omega' \text{ with } \operatorname{leb}(\Omega'') > 0 \text{ and } u|_{\Omega''} = 0 \}$$
$$\subseteq \{ u \in C(\Omega; \mathbb{R}) \mid \operatorname{leb}(u^{-1}\{0\}) > 0 \} = D'$$

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has probability zero under  $\nu_0$ . This can be deduced from Proposition 7.2 in [28]: since Assumptions 2–3 hold and  $\alpha > d$ , Theorem 4 tells us that draws from  $\nu_0$  are almost-surely continuous, which is sufficient in order to deduce the conclusions of the proposition, and so  $\nu_0(D) \le \nu_0(D') = 0$ . We thus have pointwise convergence of the integrand on  $D^c$ , and so using the boundedness of the integrand by 1 and the dominated convergence theorem,

$$\mathbb{E}^{\nu_0} e^{-\Phi_{p,1}(u;\gamma)} g(u) = \mathbb{E}^{\nu_0} e^{-\Phi_{p,1}(u;\gamma)} g(u) \mathbb{1}_{D^c}(u) \to \mathbb{E}^{\nu_0} \mathbb{1}_{B_{\infty,1}}(u) g(u)$$

which proves that  $\nu_{p,1} \Rightarrow \nu_1$ .

For the convergence  $\nu_{ls,1} \Rightarrow \nu_1$  it similarly suffices to prove that, as  $\gamma \to 0$ ,

$$\mathbb{E}^{\nu_0} e^{-\Phi_{\mathrm{ls},1}(u;\gamma)} g(u) \to \mathbb{E}^{\nu_0} \mathbb{1}_{B_{\infty,1}}(u) g(u)$$

for all continuous functions  $g: C(\Omega; \mathbb{R}) \to [-1, 1]$ . For fixed  $u \in B_{\infty,1}$  we have  $e^{-\Phi_{\mathrm{ls},1}(u;\gamma)} = \mathbb{1}_{B_{\infty,1}}(u) = 1$  and hence  $e^{-\Phi_{\mathrm{ls},1}(u;\gamma)}g(u) = \mathbb{1}_{B_{\infty,1}}(u)g(u)$  for all  $\gamma > 0$ . For fixed  $u \notin B_{\infty,1}$  there is a set  $E \subseteq \Omega'$  with positive Lebesgue measure on which  $y(x)u(x) \leq 0$ . As a consequence  $\Phi_{\mathrm{ls},1}(u;\gamma) \geq \frac{1}{2\gamma^2} \mathrm{leb}(E)\rho^-$  and so  $e^{-\Phi_{\mathrm{ls},1}(u;\gamma)}g(u) \to 0 = \mathbb{1}_{B_{\infty,1}}(u)g(u)$  as  $\gamma \to 0$ . Pointwise convergence of the integrand, combined with boundedness by 1 of the integrand, gives the result.

(ii) The structure of the proof is similar to part (i). To prove  $\nu_{p,2} \Rightarrow \nu_2$ , it suffices to show that, as  $\gamma \to 0$ ,

$$\mathbb{E}^{\nu_0} e^{-\Phi_{\mathbf{p},2}(u;\gamma)} g(u) \to \mathbb{E}^{\nu_0} \mathbb{1}_{B_{\infty,2}}(u) g(u)$$

for all continuous functions  $g: C(\Omega; \mathbb{R}) \mapsto [-1, 1]$ . We write

$$\Phi_{\mathbf{p}}^{(n)}(u;\gamma) = -\frac{1}{n} \sum_{j \in Z'} \log \Big( \varphi(y(x_j)u(x_j)/\gamma) \Big) \ge 0$$

$$e^{-\Phi_{\mathbf{p},2}(u;\gamma)}g(u) \to g(u) = \mathbb{1}_{B_{\infty,2}}(u)g(u)$$

Now suppose that  $u \notin B_{\infty,2}$ . Assume first that there is a  $j \in Z'$  such that  $y(x_j)u(x_j) < 0$ , so that  $y(x_j)u(x_j)/\gamma \to -\infty$  and hence  $\varphi(y(x_j)u(x_j)/\gamma) \to 0$ . Then we may bound

$$\Phi_{\mathrm{p},2}(u;\gamma) \ge -\log(\varphi(y(x_j)u(x_j)/\gamma) \to \infty$$

from which we see that

$$e^{-\Phi_{p,2}(u;\gamma)}g(u) \to 0 = \mathbb{1}_{B_{\infty,2}}(u)g(u)$$

Assume now that  $y(x_j)u(x_j) \ge 0$  for all  $j \in Z'$ , then since  $u \notin B_{\infty,2}$  there is a subcollection  $Z'' \subseteq Z'$  such that  $y(x_j)u(x_j) = 0$  for all  $j \in Z''$  and  $y(x_j)u(x_j) > 0$  for all  $j \in Z' \setminus Z''$ . We then have

$$\begin{split} \Phi_{\mathbf{p},2}(u;\gamma) &= -\frac{1}{n} \sum_{j \in Z''} \log\Big(\varphi(0)\Big) - \frac{1}{n} \sum_{j \in Z' \smallsetminus Z''} \log\Big(\varphi(y(x_j)u(x_j)/\gamma)\Big) \\ &= \frac{|Z''|}{n} \log(2) - \frac{1}{n} \sum_{j \in Z' \smallsetminus Z''} \log\Big(\varphi(y(x_j)u(x_j)/\gamma)\Big) \\ &\to \frac{|Z''|}{n} \log(2). \end{split}$$

Thus, in this case  $e^{-\Phi_{p,2}(u;\gamma)}g(u) \neq 0 = \mathbb{1}_{B_{\infty,2}}(u)g(u)$ . However, the event

$$D = \{ u \in C(\Omega; \mathbb{R}) \mid u(x_j) = 0 \text{ for some } j \in Z' \}$$

has probability zero under  $\nu_0$ . To see this, observe that  $\nu_0$  is a non-degenerate Gaussian measure on  $C(\Omega; \mathbb{R})$  as a consequence of Theorem 4. Thus  $u \sim \nu_0$ implies that the vector  $(u(x_1), \ldots, u(x_{n^++n^-}))$  is a non-degenerate Gaussian random variable on  $\mathbb{R}^{n^++n^-}$ . Its law is hence equivalent to the Lebesgue measure, and so the probability that it takes value in any given hyperplane is zero. We therefore have pointwise convergence of the integrand on  $D^c$ . Since the integrand is bounded by 1, we deduce from the dominated convergence theorem that 

$$\mathbb{E}^{\nu_{0}} e^{-\Phi_{\mathbf{p},2}(u;\gamma)} g(u) = \mathbb{E}^{\nu_{0}} e^{-\Phi_{\mathbf{p},2}(u;\gamma)} g(u) \mathbb{1}_{D^{c}}(u) \to \mathbb{E}^{\nu_{0}} \mathbb{1}_{B_{\infty,2}}(u) g(u)$$
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which proves that  $\nu_{p,2} \Rightarrow \nu_2$ . To prove  $\nu_{ls,2} \Rightarrow \nu_2$  we show that, as  $\gamma \to 0$ ,

$$\mathbb{E}^{\nu_0} e^{-\Phi_{\mathrm{ls},2}(u;\gamma)} g(u) \to \mathbb{E}^{\nu_0} \mathbb{1}_{B_{\infty,2}}(u) g(u)$$

1182	for all continuous functions $g: C(\Omega; \mathbb{R}) \mapsto [-1, 1]$ . For fixed $u \in B_{\infty, 2}$ we have
1183	$e^{-\Phi_{1s,2}(u;\gamma)} = \mathbb{1}_{B_{\infty,2}}(u) = 1$ and hence $e^{-\Phi_{1s,2}(u;\gamma)}g(u) = \mathbb{1}_{B_{\infty,2}}(u)g(u)$ for a
1184	$\gamma > 0$ . For fixed $u \notin B_{\infty,2}$ there is at least one $j \in Z'$ such that $y(x_j)u(x_j)$
1185	0. As a consequence $\Phi_{ls,2}(u;\gamma) \geq \frac{1}{2\gamma^2} \frac{1}{n} \rho^-$ and so $e^{-\Phi_{ls,2}(u;\gamma)} g(u) \to 0$
1186	$\mathbb{1}_{B_{\infty,2}}(u)g(u)$ as $\gamma \to 0$ . Pointwise convergence of the integrand, combine
1187	with boundedness by 1 of the integrand, gives the desired result.

<sup>1188</sup> **7.8. Technical lemmas.** We include technical lemmas which are used in the <sup>1189</sup> main Γ-convergence result (Theorem 1) and in the proof of convergence for the probit <sup>1190</sup> model.

LEMMA 24. Let X be a normed space and  $a_k^{(n)} \in X$  for all  $n \in \mathbb{N}$  and k = 1, ..., n. Assume  $a_k \in X$  be such that  $\sum_{k=1}^{\infty} ||a_k|| < \infty$  and that for all k

$$a_k^{(n)} \to a_k \quad \text{as } n \to \infty.$$

Then there exists a sequence  $\{K_n\}_{n=1,\dots}$  converging to infinity as  $n \to \infty$  such that

$$\sum_{k=1}^{K_n} a_k^{(n)} \to \sum_{k=1}^{\infty} a_k \quad \text{as } n \to \infty.$$

<sup>1194</sup> Note that if the conclusion holds for one sequence  $K_n$  it also holds for any other <sup>1195</sup> sequence converging to infinity and majorized by  $K_n$ .

Proof. Note that by our assumption for any fixed s,  $\sum_{k=1}^{s} a_k^n \to \sum_{k=1}^{s} a_k$  as  $n \to \infty$ . Let  $K_n$  be the largest number such that for all  $m \ge n$ ,  $\left\|\sum_{k=1}^{K_n} a_k^{(m)} - \sum_{k=1}^{K_n} a_k\right\| < \frac{1}{n}$ . Due to observation above,  $K_n \to \infty$  as  $n \to \infty$ . Furthermore

$$\left\|\sum_{k=1}^{K_n} a_k^n - \sum_{k=1}^{\infty} a_k\right\| \le \left\|\sum_{k=1}^{K_n} a_k^n - \sum_{k=1}^{K_n} a_k\right\| + \left\|\sum_{k=K_n+1}^{\infty} a_k\right\|$$

1199 which converges to zero an  $n \to \infty$ .

The second result is an estimate on the behavior of the function  $\Psi$  defined in (8)

LEMMA 25. Let  $F(w, v) = \log \Psi(w; 1) - \log \Psi(v; 1)$  where  $\Psi$  is defined by (8) with  $\gamma = 1$ . For all w > v and  $M \ge 1$ ,

$$F(w,v) \le \begin{cases} 2v^2 + \frac{1}{M^2} & \text{if } v \le -M \\ \frac{|w-v|}{\int_{-\infty}^{-M} e^{-\frac{t^2}{2}} dt} & \text{if } v \ge -M. \end{cases}$$

<sup>1203</sup> Proof. We consider the two cases:  $v \leq -M$  and  $v \geq -M$  separately. From inequal-<sup>1204</sup> ity 7.1.13 in [2] directly follows that

$$\forall u \le 0, \qquad \sqrt{\frac{2}{\pi}} \frac{1}{-u + \sqrt{u^2 + 4}} e^{-\frac{u^2}{2}} \le \Psi(u)$$
  
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When  $v \leq -M$ , by taking the logarithm we obtain

$$F(w,v) \le -\log \Psi(v;\gamma) \le -\log \left(\sqrt{\frac{2}{\pi}} \frac{1}{-v + \sqrt{v^2 + 4}} e^{-\frac{v^2}{2}}\right) \le \sqrt{\frac{\pi}{2}} \left(\sqrt{v^2 + 4} - v\right) + \frac{v^2}{2}$$
$$\le \sqrt{\frac{\pi}{2}} |v| \left(\sqrt{1 + \frac{4}{M^2}} - 1\right) + \frac{v^2}{2} \le \frac{\sqrt{2\pi}|v|}{M} + \frac{v^2}{2} \le 2v^2 + \frac{1}{M^2}$$

using the elementary bound  $|\sqrt{1+x^2}-1| \le |x|$  for all  $x \ge 0$ . When  $v \ge -M$ ,

$$F(w,v) = \log \frac{\Psi(w)}{\Psi(v)} = \log \left( 1 + \frac{\int_v^w e^{-\frac{t^2}{2}} dt}{\int_{-\infty}^v e^{-\frac{t^2}{2}} dt} \right) \le \frac{\int_v^w e^{-\frac{t^2}{2}} dt}{\int_{-\infty}^v e^{-\frac{t^2}{2}} dt} \le \frac{w-v}{\int_{-\infty}^{-M} e^{-\frac{t^2}{2}} dt}$$

<sup>1206</sup> This completes the proof.

1207 COROLLARY 26. Let  $\Omega' \subset \mathbb{R}^d$  be open and bounded. Let  $\mu'$  be a bounded, non-1208 negative measure on  $\Omega'$  and  $\gamma > 0$ . Define  $\Psi(\cdot; \gamma)$  as in (8). If  $v \in L^2_{\mu'}$  then 1209  $\log \Psi(v; \gamma) \in L^1(\mu')$ .

Proof. Lemma 25, and using that  $\Psi(v;\gamma) = \Psi(v|\gamma;1)$ , shows that  $-\log \Psi(v,\gamma)$ grows quadratically as  $v \to -\infty$ . Note that  $-\log \Psi(v,\gamma)$  asymptotes to zero as  $v \to \infty$ . Therefore  $|\log \Psi(v,\gamma)| \le C(|v|^2 + 1)$  for some C > 0, which implies the claim.

## <sup>1213</sup> 7.9. Weyl's Law.

LEMMA 27. Let  $\Omega$  and  $\rho$  satisfy Assumptions 2-3 and let  $\lambda_k$  be the eigenvalues of  $\mathcal{L}$  defined by (4). Then, there exist positive constants c and C such that for all klarge enough

$$ck^{\frac{2}{d}} \le \lambda_k \le Ck^{\frac{2}{d}}.$$

*Proof.* Let *B* be a ball compactly contained in  $\Omega$  and *U* a ball which compactly contains  $\Omega$ . By assumptions on  $\rho$  for all  $u \in H_0^1(B) \setminus \{0\}$ 

$$\frac{\int_{B} |\nabla u|^2 dx}{\int_{B} u^2 dx} \ge c_2 \frac{\int_{\Omega} |\nabla u|^2 \rho^2 dx}{\int_{\Omega} u^2 \rho dx}$$

where on RHS we consider the extension by zero of u to  $\Omega$ . Therefore for any kdimensional subspace  $V_k$  of  $H_0^1(B)$ 

$$\max_{u \in V_k \setminus \{0\}} \frac{\int_B |\nabla u|^2 dx}{\int_B u^2 dx} \geq c_2 \max_{u \in V_k \setminus \{0\}} \frac{\int_\Omega |\nabla u|^2 \rho^2 dx}{\int_\Omega u^2 \rho dx}$$

<sup>1221</sup> Consequently, using the Courant–Fisher characterization of eigenvalues,

$$\alpha_{k} = \inf_{\substack{V_{k} \subset H_{0}^{1}(B), \ u \in V_{k} \setminus \{0\} \\ \dim V_{k} = k}} \max_{\substack{U_{k} \subset H_{0}^{1}(\Omega), \ u \in V_{k} \setminus \{0\} \\ \dim V_{k} = k}} \frac{\int_{B} |\nabla u|^{2} dx}{\int_{B} u^{2} dx} \ge c_{2} \inf_{\substack{V_{k} \subset H^{1}(\Omega), \ u \in V_{k} \setminus \{0\} \\ \dim V_{k} = k}} \max_{\substack{U_{k} \subset H^{1}(\Omega), \ u \in V_{k} \setminus \{0\} \\ \dim V_{k} = k}} \frac{\int_{\Omega} |\nabla u|^{2} \rho^{2} dx}{\int_{\Omega} u^{2} \rho dx} = c_{2} \lambda_{k}$$

Since  $\overline{\Omega}$  is an extension domain (as it has a Lipschitz boundary), there exists an bounded extension operator  $E: H^1(\Omega) \to H^1_0(U)$ . Therefore for some constant  $C_2$  and all  $u \in H^1(\Omega)$ ,  $C_2 \int_{\Omega} |\nabla u|^2 \rho^2 + u^2 \rho dx \ge \int_U |\nabla E u|^2 dx$ . Arguing as above gives  $C_2(\lambda_k + 1) \ge \beta_k$ .

These inequalities imply the claim of the lemma, since the Dirichlet eigenvalues of the Laplacian on B,  $\alpha_k$  satisfy  $\alpha_k \leq C_1 k^{\frac{2}{d}}$  for some  $C_1$  and that Dirichlet eigenvalues of the Laplacian on U,  $\beta_k$  satisfy  $\beta_k \geq c_1 k^{\frac{2}{d}}$  for some  $c_1 > 0$ .

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