

The Evidence Framework Applied to Sparse Kernel Logistic Regression

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Abstract

In this paper we present a simple hierarchical Bayesian treatment of the sparse kernel logistic regression (KLR) model based on the evidence framework introduced by MacKay. The principal innovation lies in the re-parameterisation of the model such that the usual spherical Gaussian prior over the parameters in the kernel induced feature space also corresponds to a spherical Gaussian prior over the transformed parameters, permitting the straight-forward derivation of an efficient update formula for the regularisation parameter. The Bayesian framework also allows the selection of good values for kernel parameters through maximisation of the marginal likelihood, or evidence, for the model. Results obtained on a variety of benchmark datasets are provided indicating that the Bayesian kernel logistic regression model is competitive with kernel logistic regression models, where the hyper-parameters are selected via cross-validation and with the support vector machine and relevance vector machine.

Key words: Bayesian learning, kernel methods, logistic regression

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1 Introduction

The “kernel trick” provides a general mechanism for constructing non-linear generalisations of a wide range of conventional linear statistical methods. The resulting family of kernel learning methods has frequently demonstrated state-of-the-art performance on a wide range of bench-mark and real-world applications, while retaining the mathematical tractability of the underlying linear model (for an overview of kernel learning methods, see Cristianini and Shawe-Taylor [1] or Schölkopf and Smola [2]). The Support Vector Machine (SVM) [3–5] is arguably the best known kernel learning method for statistical pattern recognition. The support vector machine embodies the maxim that “one should solve the problem directly and never solve a more general problem as an intermediate step” [5] and so aims to estimate the optimal decision boundary separating examples belonging to each class directly, rather than estimating the *a-posteriori* probability of class membership and subsequently establishing the decision boundary at some fixed threshold probability. While this principle is entirely justifiable, there are circumstances where estimates of *a-posteriori* probability are useful, especially where the operational prior class probabilities, or equivalently the costs associated with false-positive and false-negative errors, are variable or are unknown at the time of training the classifier. Here we consider kernel logistic regression (e.g. [6]), a kernel learning method which aims to estimate the *a-posteriori* probability of class membership, based on the familiar method of logistic regression of classical statistics (e.g. [7]).

The parameters of a kernel model are typically given by the solution of a

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convex optimisation problem, and so there is a single, global optimum. The generalisation properties of kernel machines are however governed by a small number of regularisation and kernel parameters, most frequently tuned via lengthy, computationally intensive optimisation of a cross-validation based model selection criterion. In addition, although the training criterion is unimodal, there remains irreducible uncertainty in the optimal values of the model parameters inherent in estimates based on a finite sample of training data. The Bayesian approach provides an elegant solution to both of these problems, by *marginalising* over (integrating out) both the model parameters and hyper-parameters when making inferences. In this paper, we apply the Evidence framework developed by MacKay [8–10] for approximate Bayesian inference using kernel logistic regression models. Under the evidence framework, the posterior distribution over the model parameters is assumed to be Gaussian (i.e. the Laplace approximation) so that the necessary integrals can be approximated analytically. The posterior distribution over the hyper-parameters is then assumed to be sharply peaked, such that the full Bayesian inference can be reasonably well approximated using a model trained with the hyper-parameters fixed at their most probable values. A Bayesian treatment of the kernel logistic regression model, under the evidence framework, is relatively straight-forward, provided that the model is first re-parameterised so that the usual feature-space regularisation term corresponds to a spherical Gaussian prior over the transformed parameters. While this re-parameterisation is not required to form the Laplace approximation, it greatly simplifies the derivation of an efficient update formula for the regularisation parameter.

The optimisation problem to be solved in training a kernel machine usually involves one free parameter per training example, and so the computational

complexity of the training algorithm can be as high as $\mathcal{O}(\ell^3)$, where ℓ is the number of training patterns. Imposing sparsity on the vector of model parameters is therefore vital in order for the training procedure to remain computationally tractable in medium to large scale applications (presently anything above a few thousand training examples). We therefore consider Bayesian learning for sparse kernel logistic regression models. Selection of a small set of basis vectors can be achieved using a variety of practicable algorithms, including random selection [11] and greedy selection [2, 12] in addition to the incomplete Cholesky factorisation [13] used here, the emphasis of the paper is therefore on Bayesian learning *following* sparsification.

The remainder of the paper is structured as follows: The sparse kernel logistic regression model is defined in section 2, introducing the notation used throughout. Section 3 introduces a Bayesian treatment of the sparse kernel logistic regression model. Results obtained using both Bayesian and frequentist kernel logistic regression models on a variety of benchmark datasets are given in section 4. A discussion of the advantages and disadvantages of the evidence approximation and Bayesian inference using Markov Chain Monte Carlo (MCMC) methods is given in section 5, along with a comparison of the Bayesian kernel logistic regression model with the Relevance Vector Machine [14]. Finally, the work is summarised and conclusions drawn in section 6.

2 Sparse Kernel Logistic Regression

In this section, we provide a brief description of the sparse kernel logistic regression model and conventional training procedures based on the iteratively re-weighted least-squares (IRWLS) algorithm.

2.1 Logistic Regression

Assume we are given labelled training data, $\mathcal{D} = \{(\mathbf{x}_i, t_i)\}_{i=1}^{\ell}$, $\mathbf{x}_i \in \mathcal{X} \subset \mathbb{R}^d$, $t_i \in (0, 1)$, where \mathbf{x}_i the vector of input features describing the i^{th} example and t_i represents the probability that the i^{th} example belongs to class \mathcal{C}_1 rather than class \mathcal{C}_2 , most commonly $t_i \in \{0, 1\}$. The logistic regression procedure (e.g. [7]) aims to construct a linear model of the form

$$\text{logit}\{y(\mathbf{x}; \mathbf{w}, b)\} = \mathbf{w} \cdot \mathbf{x} + b \quad \text{where} \quad \text{logit}\{p\} = \log \left\{ \frac{p}{1-p} \right\},$$

the output of which can be interpreted as an estimate of the *a-posteriori* probability of class membership, i.e. $y(\mathbf{x}) \approx p(t = 1|\mathbf{x})$. Assuming the target, t_i , represents an independent and identically distributed (i.i.d.) sample drawn from a Bernoulli distribution conditioned on the input vector, \mathbf{x}_i , the *likelihood* of the data is given by

$$\mathcal{L}_{\mathcal{D}} = \prod_{i=1}^{\ell} (y_i)^{t_i} (1 - y_i)^{1-t_i}$$

where $y_i = y(\mathbf{x}_i; \mathbf{w}, b)$. The optimal model parameters $\boldsymbol{\omega} = (\mathbf{w}, b)$, are then determined by minimising the negative logarithm of the likelihood, in this case known as the *cross-entropy*,

$$E(\mathbf{w}, b) = - \sum_{i=1}^{\ell} \{t_i \log y_i + (1 - t_i) \log(1 - y_i)\}.$$

The bias term, b , can be implemented most conveniently by augmenting the input vector to contain an additional feature with a fixed constant value for all patterns. Let $\mathbf{X} = [\mathbf{x}_i]_{i=1}^{\ell}$ represent the matrix, where each row is given by one of the ℓ input vectors comprising \mathcal{D} . Furthermore, let $\boldsymbol{\Phi} = [\mathbf{X} \mathbf{1}]$, where $\mathbf{1}$ represents a column vector of ℓ ones. The optimal vector of model parameters, $\boldsymbol{\omega}$, can then be found efficiently via the iteratively re-weighted least-squares

(IRWLS) procedure: At each iteration, the model parameters are given by the solution of a weighted least-squares problem, such that

$$\boldsymbol{\omega} = \left(\boldsymbol{\Phi}^T \mathbf{W} \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^T \mathbf{W} \boldsymbol{\eta}, \quad (1)$$

where $\mathbf{W} = \text{diag}(\{w_1, w_2, \dots, w_\ell\})$ is a diagonal weight matrix with non-zero elements given by

$$w_i = y_i(1 - y_i), \quad \forall i \in \{1, 2, \dots, \ell\} \quad (2)$$

and $\boldsymbol{\eta} = (\eta_1, \eta_2, \dots, \eta_\ell)$ given by

$$\eta_i = z_i + \frac{t_i - y_i}{y_i(1 - y_i)}, \quad \forall i \in \{1, 2, \dots, \ell\} \quad (3)$$

where $z_i = \text{logit}\{y_i\}$. The algorithm proceeds iteratively, updating the weights according to (1) and then updating \mathbf{W} and $\boldsymbol{\eta}$ according to (2) and (3) until convergence is achieved.

2.2 Kernel Logistic Regression

A non-linear form of logistic regression, known as Kernel Logistic Regression (KLR), can be constructed using the familiar “kernel trick” (e.g. [6]). Let \mathcal{F} represent a feature space corresponding to a fixed transformation of the input space, $\boldsymbol{\phi} : \mathcal{X} \rightarrow \mathcal{F}$. The kernel logistic regression model implements a conventional linear logistic regression model in the feature space,

$$\text{logit}\{y(\mathbf{x}; \mathbf{w})\} = \mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x}),$$

note that, for the sake of notational convenience, we omit the bias term, b , however a bias was included in our implementation. Due to the non-linear action of the kernel, a linear model in \mathcal{F} appears as a non-linear model in the

input space, \mathcal{X} . However, rather than defining the feature space explicitly, it is instead defined by a kernel function, $\mathcal{K} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, that evaluates the inner product between the images of input vectors in the feature space, i.e. $\mathcal{K}(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x}) \cdot \boldsymbol{\phi}(\mathbf{x}')$. For a kernel to support the interpretation as an inner product in a fixed feature space, the kernel must obey Mercer's condition [15], that is the Gram matrix for the kernel, $\mathbf{K} = [k_{ij} = \mathcal{K}(\mathbf{x}_i, \mathbf{x}_j)]_{i,j=1}^{\ell}$, must be positive semi-definite. Provided that the training procedure can be formulated such the input vectors, \mathbf{x}_i , appear only in the form of inner products, this allows the use of very high dimensional feature spaces, resulting in very flexible, powerful models. The Radial Basis Function (RBF) kernel is perhaps the most commonly encountered kernel,

$$\mathcal{K}(\mathbf{x}, \mathbf{x}') = \exp \left\{ \zeta \|\mathbf{x} - \mathbf{x}'\|^2 \right\}, \quad (4)$$

where ζ is a *kernel parameter* controlling the sensitivity of the kernel. In this case, $\boldsymbol{\phi}$ maps vectors from \mathcal{X} onto one quadrant of an infinite-dimensional unit hyper-sphere [2].

When constructing a statistical model in a high-dimensional space, as is the case here, it is prudent to take steps to avoid over-fitting the training data. As a result, the kernel logistic regression model is trained using a *regularised* [16] cross-entropy loss function,

$$E(\mathbf{w}, b) = - \sum_{i=1}^{\ell} \{ t_i \log y_i + (1 - t_i) \log(1 - y_i) \} + \frac{\mu}{2} \|\mathbf{w}\|^2, \quad (5)$$

where μ is a *regularisation parameter* controlling the bias-variance trade-off [17]. The representer theorem [18, 19] states that the solution of an optimisation criterion of the form (5) can be expressed in the form of an expansion

over training patterns,

$$\mathbf{w} = \sum_{i=1}^{\ell} \alpha_i \phi(\mathbf{x}_i), \quad (6)$$

and so we have

$$\text{logit}\{y(\mathbf{x}; \boldsymbol{\alpha})\} = \sum_{i=1}^{\ell} \alpha_i \mathcal{K}(\mathbf{x}_i, \mathbf{x}) \quad \text{and} \quad \|\mathbf{w}\|^2 = \boldsymbol{\alpha}^T \mathbf{K} \boldsymbol{\alpha}.$$

The optimal value for the vector of “dual” model parameters, $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_\ell)$, can again be found via a simple iteratively re-weighted least squares procedure.

2.3 Imposing Sparsity

A major disadvantage of kernel learning methods is that the kernel expansion contains one coefficient for each training pattern. This is clearly impractical for applications with more than a few thousands of examples, as the computational complexity of the training algorithm is often as high as $\mathcal{O}(\ell^3)$ as, for example, in the case of the iteratively re-weighted least-squares procedure. The solution to this problem is to approximate the full kernel expansion (6) by an expansion over a limited subset of the training patterns, known as *representers*,

$$\mathbf{w} = \sum_{i=1}^N \alpha_i \phi(\mathbf{x}_i), \quad \implies \quad \text{logit}\{y(\mathbf{x}; \boldsymbol{\alpha})\} = \sum_{i=1}^N \alpha_i \mathcal{K}(\mathbf{x}_i, \mathbf{x}),$$

where for notational convenience we assume that only the first N training patterns are included in the kernel expansion. The vector of model parameters, $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_N)$, of a sparse kernel logistic regression model is then given by the minimum of a regularised cross-entropy criterion,

$$E(\boldsymbol{\alpha}) = \sum_{i=1}^{\ell} C\{t_i, y(\mathbf{x}_i; \boldsymbol{\alpha})\} + \frac{\mu}{2} \boldsymbol{\alpha}^T \tilde{\mathbf{K}} \boldsymbol{\alpha}, \quad (7)$$

where $C\{t, y\} = -t \log y - (1 - t) \log(1 - y)$ and $\hat{\mathbf{K}} = [\hat{k}_{ij} = \mathcal{K}(\mathbf{x}_i, \mathbf{x}_j)]_{i,j=1}^N$ is a square sub-matrix of the Gram matrix. There are many ways in which to select terms to include in the sparse kernel expansion, the simplest being to choose a random subset of training patterns. Alternatively, one could iteratively introduce terms in a greedy manner, so as to produce the greatest decrease in the training criterion (c.f. [2, 12]). The Gram matrix, \mathbf{K} for a radial basis function kernel is at least in principle of full rank, assuming that $\mathbf{x}_i \neq \mathbf{x}_j, \forall i, j \in \{1, 2, \dots, \ell\}$ [20]; however it is possible for \mathbf{K} to be *numerically* rank-deficient. A third alternative is therefore to identify a linearly independent subset of columns forming an approximate basis for the entire Gram matrix. The remaining columns are linearly dependent, or close to being linearly dependent, on the columns selected to form the basis and the corresponding terms can safely be omitted from the kernel expansion [21]. In this study, the selection of an approximate basis is achieved via the the incomplete Cholesky factorisation with symmetric pivoting, due to Fine and Scheinberg [13].

In general, the numerical rank deficiency of the kernel is likely to be lowest for highly non-linear kernels, for instance RBF kernels with large values for ζ . A higher degree of sparsity can therefore be obtained using simple kernels, such as an RBF kernel with a small value of ζ . In the case of an RBF kernel, experiments also suggest that a dataset with a small number of input variables (i.e. $\ell \gg d$) will result in a greater degree of sparsity than a dataset with many input variables. It should be noted however that one might seek to continue to prune representers after the kernel matrix has already been made of full numeric rank. In this case, the resulting model will only *approximate* the full kernel logistic regression model, rather than being functionally equivalent. In

this case, the incomplete Cholesky factorisation can be used to rank training patterns for use as representers.

3 Sparse Bayesian Kernel Logistic Regression

The application of the evidence framework to sparse kernel logistic regression is relatively straight-forward, except for the derivation of an efficient update formula for the regularisation parameter μ (see section 3.2), which requires the Hessian of the training criterion with respect to the model parameters to be of the form $\mathbf{H} + \mu\mathbf{I}$, where \mathbf{I} is the identity matrix and \mathbf{H} is independent of μ . This would be the case if we were to apply a weight-decay regularisation term [22, 23] to the coefficients of the expansion, i.e.

$$L(\boldsymbol{\alpha}) = \sum_{i=1}^{\ell} C\{t_i, y(\mathbf{x}_i; \boldsymbol{\alpha})\} + \frac{\mu}{2} \|\boldsymbol{\alpha}\|^2,$$

however the use of a feature space regularisation term, $\|\mathbf{w}\|^2$, means that we end up with a Hessian of the form $\mathbf{H} + \mu\hat{\mathbf{K}}$ and the usual derivation is no longer possible. We therefore begin by re-parameterising our model such that the feature-space regularisation term is replaced by a simple weight-decay regulariser acting on the transformed parameters, i.e. $\boldsymbol{\alpha}^T \mathbf{K} \boldsymbol{\alpha} = \boldsymbol{\beta}^T \boldsymbol{\beta} = \|\boldsymbol{\beta}\|^2$, where $\boldsymbol{\beta}$ is the vector of transformed parameters. Let \mathbf{R} represent the upper triangular Cholesky factor [24] of the symmetric positive-definite matrix $\hat{\mathbf{K}}$, such that $\hat{\mathbf{K}} = \mathbf{R}^T \mathbf{R}$. By inspection, the desired parameterisation is given then by

$$\boldsymbol{\beta} = \mathbf{R}\boldsymbol{\alpha} \quad \implies \quad \boldsymbol{\alpha} = \mathbf{R}^{-1}\boldsymbol{\beta}.$$

We then proceed with the Bayesian analysis using the transformed parameters, with the re-parameterised training criterion,

$$L(\boldsymbol{\beta}) = \sum_{i=1}^{\ell} C\{t_i, y(\mathbf{x}_i; \boldsymbol{\beta})\} + \frac{\mu}{2} \boldsymbol{\beta}^T \boldsymbol{\beta} = E_{\mathcal{D}} + \frac{\mu}{2} E_{\beta}, \quad (8)$$

where $E_{\mathcal{D}}$ and E_{β} represent the components due to the data misfit and regularisation terms respectively, and the output of the re-parameterised model is given by

$$\text{logit}\{y(\mathbf{x}; \boldsymbol{\beta})\} = \mathbf{k}^T(\mathbf{x}) \mathbf{R}^{-1} \boldsymbol{\beta}, \quad \text{where} \quad \mathbf{k}(\mathbf{x}) = [\mathcal{K}(\mathbf{x}_i, \mathbf{x})]_{i=1}^N.$$

Again the optimal model parameters, $\boldsymbol{\beta}$, can be determined via the IRWLS procedure. This is essentially the only innovation required to formulate a Bayesian kernel logistic regression model under the evidence framework. It is important to note that all we have done is to re-parameterise the model, the training criteria (7) and (8) are exactly equivalent.

3.1 Bayesian Interpretation of the Training Criterion

In the remainder of this section, we briefly summarise the Bayesian methods introduced by MacKay [8–10], based on the lucid exposition provided by Bishop [23]. Minimising the criterion given in equation (8) is equivalent to maximising the posterior distribution

$$p(\boldsymbol{\beta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\beta})p(\boldsymbol{\beta}|\mu)}{p(\mathcal{D})} \quad (9)$$

where the likelihood is given by the Bernoulli distribution

$$p(\mathcal{D}|\boldsymbol{\beta}) = \prod_{i=1}^{\ell} y(\mathbf{x}_i; \boldsymbol{\beta})^{t_i} [1 - y(\mathbf{x}_i; \boldsymbol{\beta})]^{(1-t_i)},$$

and the prior over model parameters by a multivariate Gaussian distribution,

$$p(\boldsymbol{\beta}) = \left[\frac{\mu}{2\pi} \right]^{N/2} \exp \left\{ -\frac{\mu}{2} \|\boldsymbol{\beta}\|^2 \right\}.$$

The Taylor series expansion of $L(\boldsymbol{\beta}, \mu)$ around the most probable value, $\boldsymbol{\beta}^{\text{MP}}$, gives rise to familiar Gaussian approximation to the posterior distribution, known as the ‘‘Laplace approximation’’,

$$p(\boldsymbol{\beta}|\mathcal{D}) \approx \frac{1}{Z^*} \exp \left\{ -L(\boldsymbol{\beta}^{\text{MP}}) - \frac{1}{2} \Delta\boldsymbol{\beta}^T \mathbf{A} \Delta\boldsymbol{\beta} \right\}, \quad (10)$$

where Z^* is an appropriate normalising constant, $\Delta\boldsymbol{\beta} = \boldsymbol{\beta} - \boldsymbol{\beta}^{\text{MP}}$ and $\mathbf{A} = \nabla\nabla L(\boldsymbol{\beta}) = \nabla\nabla E_{\mathcal{D}} + \mu\mathbf{I}$ is the Hessian of $L(\boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}$, evaluated at $\boldsymbol{\beta}^{\text{MP}}$.

3.1.1 Marginalising over Model Parameters

The posterior distribution over the model parameters describes the uncertainty in estimating the model parameters from a finite set of training patterns. The Bayesian approach seeks to integrate out the model parameters when making inferences in order to account for the uncertainty in estimating the model parameters, such that

$$p(\mathcal{C}_1|\mathbf{x}, \mathcal{D}) = \int p(\mathcal{C}_1|\mathbf{x}, \boldsymbol{\beta})p(\boldsymbol{\beta}|\mathcal{D})d\boldsymbol{\beta}.$$

This process is known as *marginalisation*. Let $a = \text{logit}\{y(\mathbf{x}; \boldsymbol{\beta})\}$: As a is a linear function of the model parameters, $\boldsymbol{\beta}$, the Laplace approximation implies that a also has a Gaussian distribution, centred on the most probable value, a_{MP} ,

$$p(a|\mathbf{x}, \mathcal{D}) = \frac{1}{\sqrt{2\pi}s} \exp \left\{ -\frac{(a - a_{\text{MP}})^2}{2s^2} \right\},$$

with variance $s^2 = \mathbf{g}^T \mathbf{A}^{-1} \mathbf{g}$, where \mathbf{g} is the first derivative of a , with respect to $\boldsymbol{\beta}$, evaluated at $\boldsymbol{\beta}^{\text{MP}}$. Rather than marginalise over $\boldsymbol{\beta}$, we may equivalently marginalise over a , the probability that a pattern, \mathbf{x} , belongs to class \mathcal{C}_1 can then be written as

$$p(\mathcal{C}_1 | \mathbf{x}, \mathcal{D}) = \int p(\mathcal{C}_1 | a) p(a | \mathbf{x}, \mathcal{D}) da = \int g(a) p(a | \mathbf{x}, \mathcal{D}) da, \quad (11)$$

where $g(a) = 1/[1 + \exp(-a)]$. The integral (11) is not analytically tractable, and so MacKay [10] suggests the following approximation,

$$p(\mathcal{C}_1; \mathbf{x}, \mathcal{D}) \approx g(\kappa(s)a_{\text{MP}}) \quad \text{where} \quad \kappa(s) = \left(1 + \frac{\pi s^2}{8}\right)^{-\frac{1}{2}}.$$

3.2 The Evidence Approximation for μ

The evidence approximation [8–10] assumes that the posterior distribution for the regularisation parameter, $p(\mu | \mathcal{D})$, is sharply peaked about its most probable value, μ^{MP} , suggesting the following approximation to the posterior distribution for $\boldsymbol{\beta}$,

$$p(\boldsymbol{\beta} | \mathcal{D}) = \int p(\boldsymbol{\beta} | \mu, \mathcal{D}) p(\mu | \mathcal{D}) d\mu \approx p(\boldsymbol{\beta} | \mu^{\text{MP}}, \mathcal{D}).$$

Thus, rather than integrate out the regularisation parameter entirely (e.g. Buntine and Weigend [25]), we simply proceed with the analysis using the regularisation parameter fixed at its most likely value. For a discussion of the validity of this approach, see MacKay [26]. We seek therefore to maximise the posterior distribution,

$$p(\mu | \mathcal{D}) = \frac{p(\mathcal{D} | \mu) p(\mu)}{p(\mathcal{D})}.$$

If the prior, $p(\mu)$ is relatively insensitive to the value of μ , then maximising the posterior is approximately equivalent to maximising the likelihood term,

$p(\mathcal{D}|\mu)$, known as the *evidence* for μ . Adopting the Gaussian approximation to the posterior for the model parameters, the log-evidence is given by

$$\log p(\mathcal{D}|\mu) = -E_{\mathcal{D}}^{\text{MP}} - \mu E_{\beta}^{\text{MP}} - \frac{1}{2} \log |\mathbf{A}| + \frac{N}{2} \log \mu. \quad (12)$$

Noting that $\mathbf{A} = \mathbf{H} + \mu \mathbf{I}$, where \mathbf{H} is the Hessian of $E_{\mathcal{D}}$ with respect to β , if the eigenvalues of \mathbf{H} are $\lambda_1, \lambda_2, \dots, \lambda_N$, then the eigenvalues of \mathbf{A} are $(\lambda_1 + \mu), (\lambda_2 + \mu), \dots, (\lambda_N + \mu)$. The derivative of $\log |\mathbf{A}|$ with respect to μ (assuming that the eigenvalues of \mathbf{H} are independent of μ) is then given by

$$\frac{d}{d\mu} \log |\mathbf{A}| = \frac{d}{d\mu} \log \left\{ \prod_{i=1}^N (\lambda_i + \mu) \right\} = \sum_{i=1}^N \frac{1}{\lambda_i + \mu}.$$

Setting the derivative of the log-evidence with respect to μ to zero, we have

$$2\mu E_{\beta}^{\text{MP}} = N - \sum_{i=1}^N \frac{\mu}{\lambda_i + \mu} = \sum_{i=1}^N \frac{\lambda_i}{\lambda_i + \mu} = \gamma,$$

where γ is the number of well determined parameters in the model. This leads to a simple update formula for the regularisation parameter:

$$\mu^{\text{new}} = \frac{\gamma}{2E_{\beta}^{\text{MP}}}. \quad (13)$$

The training procedure then alternates between updates of the primary model parameters using the IRWLS procedure and updates of the regularisation parameter according to equation (13). Note that while the re-parameterisation is not required in order to form the Laplace approximation, it is necessary for the derivation of the update formula for the regularisation parameter given in this section.

3.3 Bayesian Selection of Kernel Parameters

The evidence framework provides an efficient means of estimating good values for the regularisation parameter, μ , however there remains a need for some method to select good values for any kernel parameters. In this study, we adopt an approach based on Bayesian model comparison. Say we have a collection of models \mathcal{H} , where in this case different models correspond to different choices of the values of the kernel parameters, or even different kernel functions. It seems sensible to choose the model, \mathcal{H}_i , that maximises the posterior probability over \mathcal{H} ,

$$p(\mathcal{H}_i|\mathcal{D}) = \frac{p(\mathcal{D}|\mathcal{H}_i)p(\mathcal{H}_i)}{p(\mathcal{D})},$$

where $p(\mathcal{D}|\mathcal{H}_i)$ is known as the marginal likelihood, or *evidence* for model \mathcal{H}_i . If we have no *a-priori* reason to choose one model over another, then the prior, $p(\mathcal{H}_i)$, and the denominator are the same for every model, and so model selection can be performed based solely on the evidence. In practice it is normally preferable to consider the log-evidence, which in this case is given by

$$\log p(\mathcal{D}|\mathcal{H}_i) = -E_{\mathcal{D}}^{\text{MP}} - \mu^{\text{MP}} E_{\beta}^{\text{MP}} - \frac{1}{2} \log |\mathbf{A}| + \frac{N}{2} \log \mu^{\text{MP}} + \frac{1}{2} \log \left(\frac{2}{\gamma} \right). \quad (14)$$

The derivation of this expression is somewhat lengthy, the interested reader is directed to the in-depth discussion of Bayesian model comparison (in the context of multi-layer perceptron networks) given in Bishop [23].

3.4 Computational Complexity

As the Bayesian learning algorithm is independent of the means of inducing sparsity, it is sensible to consider the computational complexity of each step separately. The computational expense of the iteratively re-weighted least-squares training procedure is dominated by the construction of $\Phi^T \mathbf{W} \Phi$, with a computational complexity of $\mathcal{O}(\ell N^2)$ and $\mathcal{O}(\ell N)$ storage, and solution of the normal equations (via Cholesky factorisation), with a computational complexity of $\mathcal{O}(N^3)$ per iteration and $\mathcal{O}(N^2)$ storage. The main computational expense in updating the regularisation parameter lies in computing the eigenvalues of the Hessian of $E_{\mathcal{D}}$ with respect to the model parameters, with complexity $\mathcal{O}(N^3)$ and storage $\mathcal{O}(N^2)$. The number of iterations required by the iteratively re-weighted least-squares procedure and for convergence of the regularisation parameter to its most probable value are not strongly dependent on the number of training patterns. Since $\ell \geq N$, this means that the computational complexity of the Bayesian learning scheme is $\mathcal{O}(\ell N^2)$ with storage requirements of $\mathcal{O}(\ell N)$. The computational complexity of the incomplete Cholesky factorisation is also $\mathcal{O}(\ell N^2)$, however other approaches are viable. Selecting N training patterns at random is practicable, and essentially incurs no extra computational expense, however the approximation of the full kernel logistic regression model would be likely to be poor. Alternatively, a greedy selection of training patterns in order to maximise the model evidence would be more computationally expensive, but would give a better approximation using fewer basis vectors.

4 Results

Figure 1 shows the (unmoderated) output of a Bayesian kernel logistic regression model, based on an isotropic radial basis function kernel (refeqn:rbf), for the synthetic dataset described by Ripley [27]. The regularisation parameter, μ , was optimised via the update formula given by equation (13); the kernel parameter, ζ , was selected by maximising the marginal likelihood (14) via a simple line search procedure. Clearly Bayesian kernel logistic regression is able to form a good model of the data, with little sign of over-fitting.

[Fig. 1 about here.]

4.1 Generalisation and Computational Expense

Table 2 presents the test set cross-entropy and error rate over nine datasets for Bayesian and conventional kernel logistic regression models. The datasets are from the suite of benchmarks used in the study by Rätsch *et al.* [28], and the same set of 100 random partitions of the data into training and test sets were used here. The results show the mean for each statistic over the 100 realisations of the benchmark, along with the standard error of the mean. An isotropic radial basis function kernel (4) was used in all experiments in the remainder of this section. The IRWLS training procedure was set to terminate when the relative decrease in the regularised loss function fell below a threshold of 1×10^{-9} . The regularisation and kernel parameters for the conventional kernel logistic regression models were determined in each realisation of the data by minimisation of a ten-fold cross-validation [29] estimate of the cross-entropy criterion. The value of kernel parameter for the Bayesian kernel logistic

regression model was determined via maximisation of the marginal likelihood (14), terminating when the relative difference in the marginal likelihood fell below 1×10^{-9} or the relative difference in the value of the regularisation parameter fell below 1×10^{-3} . In each case a hierarchical grid-based search heuristic was applied, on a logarithmic scale, which at the top level examined values of $\log_2 \zeta$ and (where appropriate) $\log_2 \mu$ ranging from -12 to +4 in increments of +2, this range of values was found to include the optimal hyper-parameters for all datasets. In the two successive levels of the hierarchical search, the neighbourhood of the optimal combination of hyper-parameter values from the previous level was subjected to a refined grid-search with the same number of points, but with a step-size four times smaller. Note that the differences in performance between the Bayesian and conventional kernel logistic regression model are generally quite small. However the model selection process under the Bayesian approach is less computationally demanding as the regularisation parameter is optimised by an efficient update formula. This is reflected in the model selection times shown in Table 3, which clearly favour the Bayesian approach. Note that the tolerance parameter of the incomplete Cholesky factorisation was set such that the linearly dependent representers were eliminated, while leaving the kernel logistic regression problem essentially unaltered. As a result, the number of representers is high for both Bayesian and cross-validation based model selection strategies.

[Table 1 about here.]

[Table 2 about here.]

[Table 3 about here.]

4.2 Sparsity

The results presented in the previous section were obtained using kernel logistic regression models, where just enough sparsity was introduced in order to eliminate numerical rank deficiency of the kernel matrix. In this section, we consider sparse Bayesian logistic regression models where the degree of sparsity is chosen via maximisation of the evidence for the model. The incomplete Cholesky factorisation was used to rank the representer vectors, and the number selected to form the kernel expansion chosen along with the kernel width parameter via a simple hierarchical grid-based search procedure as before. The results are shown in table 4, which also gives results for the support vector machine [3–5] and the relevance vector machine [14]. Only the first 10 random partitions of the data into training and test sets for the banana, breast cancer, titanic, waveform, german and image benchmarks were used, following the experimental procedure used by Tipping [14]. All three algorithms exhibit broadly similar performance in terms of mean test set error, and while both the RVM and BKLR generally employ fewer representer vectors than the SVM, neither the RVM nor the BKLR consistently out-perform the other in terms of sparsity. It is possible that a greedy algorithm that selects representer vectors so as to maximise the evidence would result in a greater degree of sparsity, however this has not yet been investigated.

[Table 4 about here.]

5 Discussion

In this section we discuss alternative approaches to marginalisation, which form the basic mechanism of Bayesian inference, and also compare the proposed Bayesian kernel logistic regression model with a similar Bayesian learning algorithm, namely the Relevance Vector Machine.

5.1 Approaches to Marginalisation

Two approaches to marginalisation are commonly encountered in Bayesian statistics, the Laplace approximation adopted here, where the posterior is assumed to be Gaussian, and approaches based on Markov Chain Monte Carlo (MCMC) methods [30]. Both of these approaches have been found to be viable in the context of multi-layer perceptron networks [8–10, 31]. In the case of sparse kernel logistic regression, the regularised loss function (8) is log-concave and so, unlike the multi-layer perceptron network, the posterior, $p(\boldsymbol{\beta}|\mathcal{D}, \mu)$, is unimodal. As noted by Tipping [14] log-concavity also implies that the tails of the posterior are no heavier than $\exp(-|\beta|)$, and so approximating the true posterior by a Gaussian, with relatively light tails, is not unreasonable. Further work is however needed to determine whether a more accurate integration over the model parameters and hyper-parameters via MCMC methods is justified by improved performance. Variational methods [32, 33] and Expectation propagation [34] also provide other alternative approaches worthy of further investigation.

5.2 Relationship to the Relevance Vector Machine

The Relevance Vector Machine (RVM) [14], in a statistical pattern recognition setting, constructs a model of a form identical to that of the kernel logistic regression algorithm. Like the Bayesian kernel logistic regression model, the parameters of the RVM are also determined using an hierarchical Bayesian treatment based on the Laplace approximation with the hyper-parameters set to their most probable values under the evidence framework. The difference between the two algorithms lies principally in the specification of the priors. Rather than adopting a single Gaussian prior over all of the model parameters with a single hyper-parameter, the RVM applies an Automatic Relevance Determination (ARD) prior [31, 35], where each weight has a Gaussian prior with a distinct hyper-parameter. Evidence-based tuning of these hyper-parameters generally results in the hyper-parameters of less informative basis functions becoming very large. This in turn forces the value of the corresponding weights essentially to zero, allowing redundant basis functions to be identified and pruned from the model. This is appealing as sparsity arises quite naturally as a consequence of a reasonable Bayesian prior over the model parameters. The RVM, however is not a true kernel learning method as the interpretation as a linear model constructed in a fixed feature space is lost, along with the consequent mathematical elegance and analytic tractability. The prior used in the Bayesian kernel logistic regression model corresponds to a prior over functions from a reproducing kernel Hilbert space (RKHS) defined by a Mercer kernel [2, 36]. This is beneficial as it is more natural to place a prior over the *function*, rather than merely the *parameterisation* of the model. The regression error bars for the RVM have the counter-intuitive property that they do not become

broad away from the training data [14, Appendix D.1]. This is likely to reduce the benefit of *moderating* the output of the classifier to account for the uncertainty in specifying the model parameters (see Section 3.1.1). If the operational priors are significantly different from the training set priors, or equivalently the misclassification costs are unknown or variable, this might have an impact on the operational performance of the classifier (note that situations of this nature provided the original motivation for this study). However, as revealed in the experimental results presented in the previous section, neither model is demonstrably superior in terms of generalisation, and both algorithms remain interesting as they offer subtly different approaches to the same problem.

6 Conclusions

In this paper we have proposed a simple hierarchical Bayesian treatment of the kernel logistic regression model. The Bayesian approach is found to be competitive with conventional kernel logistic regression, but greatly simplifies model selection process. The key feature of this approach is that the model is re-parameterised such that an isotropic Gaussian prior over model parameters is obtained, facilitating straight-forward implementation of MacKay’s evidence approximation via standard methods. Experimental results indicate that the Bayesian kernel logistic regression model is competitive with kernel logistic regression models using a conventional cross-validation based model selection process, and with the support vector machine and relevance vector machine. Note that this approach is quite general and could easily be applied to any kernel model minimising a regularised likelihood criterion.

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References

- [1] N. Cristianini and J. Shawe-Taylor. *An Introduction to Support Vector Machines (and other kernel-based learning methods)*. Cambridge University Press, Cambridge, U.K., 2000.
- [2] B. Schölkopf and A. J. Smola. *Learning with kernels — support vector machines, regularization, optimization and beyond*. MIT Press, Cambridge, MA, 2002.
- [3] B. E. Boser, I. M. Guyon, and V. Vapnik. A training algorithm for optimal margin classifiers. In D. Haussler, editor, *Proceedings of the fifth Annual ACM Workshop on Computational Learning Theory*, pages 144–152, Pittsburgh, PA, July 1992.
- [4] C. Cortes and V. Vapnik. Support vector networks. *Machine Learning*, 20:273–297, 1995.
- [5] V. Vapnik. *Statistical Learning Theory*. John Wiley and Sons, New York, 1998.
- [6] S. S. Keerthi, K. Duan, S. K. Shevade, and A. N. Poo. A fast dual algorithm for kernel logistic regression. In *Proceedings of the Nineteenth International Conference on Machine Learning*, pages 299–306, 8–12 July 2002.
- [7] P. McCullagh and J. A. Nelder. *Generalized linear models*, volume 37 of *Monographs on Statistics and Applied Probability*. Chapman and Hall, second edition, 1989.

- [8] D. J. C. MacKay. Bayesian interpolation. *Neural Computation*, 4(3):415–447, 1992.
- [9] D. J. C. MacKay. A practical Bayesian framework for backprop networks. *Neural Computation*, 4(3):448–472, 1992.
- [10] D. J. C. MacKay. The evidence framework applied to classification networks. *Neural Computation*, 4(5):720–736, 1992.
- [11] R. Rifkin. *Everything old is new again: A fresh look at historical approaches in machine learning*. PhD thesis, Massachusetts Institute of Technology, Cambridge, MA, USA, 2002.
- [12] G. C. Cawley and N. L. C. Talbot. A greedy training algorithm for sparse least-squares support vector machines. In *Proceedings of the International Conference on Artificial Neural Networks (ICANN-2002)*, volume 2415 of *Lecture Notes in Computer Science (LNCS)*, pages 681–686, Madrid, Spain, August 27–30 2002. Springer.
- [13] S. Fine and K. Scheinberg. Efficient SVM training using low-rank kernel representations. *Journal of Machine Learning Research*, 2:243–264, December 2001.
- [14] M. E. Tipping. Sparse Bayesian learning and the relevance vector machine. *Journal of Machine Learning Research*, 1:211–244, 2001.
- [15] J. Mercer. Functions of positive and negative type and their connection with the theory of integral equations. *Philosophical Transactions of the Royal Society of London, A*, 209:415–446, 1909.
- [16] A. N. Tikhonov and V. Y. Arsenin. *Solutions of ill-posed problems*. John Wiley, New York, 1977.
- [17] S. Geman, E. Bienenstock, and R. Doursat. Neural networks and the bias/variance dilemma. *Neural Computation*, 4(1):1–58, 1992.

- [18] G. S. Kimeldorf and G. Wahba. Some results on Tchebycheffian spline functions. *Journal of Mathematical Analysis and Applications*, 33:82–95, 1971.
- [19] B. Schölkopf, R. Herbrich, and A. J. Smola. A generalised representer theorem. In *Proceedings of the Fourteenth International Conference on Computational Learning Theory*, pages 416–426, Amsterdam, the Netherlands, July 16–19 2001.
- [20] C. A. Micchelli. Interpolation of scattered data: Distance matrices and conditionally positive definite functions. *Constructive Approximation*, 2:11–22, 1986.
- [21] G. Baudat and F. Anouar. Kernel-based methods and function approximation. In *Proceedings of the INNS/IEEE International Joint Conference on Neural Networks*, pages 1244–1249, Washington, DC, 15–19 July 2001.
- [22] A. Krogh and J. A. Hertz. A simple weight decay can improve generalization. In J. E. Moody, S. J. Hanson, and R. P. Lippmann, editors, *Advances in Neural Information Processing Systems*, volume 4, pages 950–957. Morgan Kaufmann, 1992.
- [23] C. M. Bishop. *Neural Networks for Pattern Recognition*. Oxford University Press, 1995.
- [24] G. H. Golub and C. F. Van Loan. *Matrix Computations*. The Johns Hopkins University Press, Baltimore, third edition edition, 1996.
- [25] W. L. Buntine and A. S. Weigend. Bayesian back-propagation. *Complex Systems*, 5:603–643, 1991.
- [26] D. J. C. MacKay. Hyperparameters : optimise or integrate out? In G. Heidbreder, editor, *Maximum Entropy and Bayesian Methods*. Kluwer, 1994.
- [27] B. D. Ripley. *Pattern recognition and neural networks*. Cambridge University Press, 1996.

- [28] G. Rätsch, T. Onoda, and K.-R. Müller. Soft margins for AdaBoost. *Machine Learning*, 42(3):287–320, 2001.
- [29] M. Stone. Cross-validatory choice and assessment of statistical predictions. *Journal of the Royal Statistical Society, B*, 36(1):111–147, 1974.
- [30] W. R. Gilks, S. Richardson, and D. J. Spiegelhalter. *Markov Chain Monte Carlo in practice*. Interdisciplinary Statistics. Chapman and Hall/CRC, 1996.
- [31] R. M. Neal. *Bayesian learning for neural networks*. Lecture Notes in Statistics. Springer-Verlag, New York, 1996.
- [32] M. I. Jordan, Z. Ghahramani, T. S. Jaakkola, and L. K. Saul. An introduction to variational methods for graphical models. In M. I. Jordan, editor, *Learning in Graphical Models*, Adaptive Computation and Machine Learning, pages 105–161. MIT Press, 1998.
- [33] T. S. Jaakkola and M. I. Jordan. Bayesian parameter estimation through variational methods. *Statistics and Computing*, 10(25–37), 2000.
- [34] T. P. Minka. *A family of algorithms for approximate Bayesian inference*. PhD thesis, Massachusetts Institute of Technology, Cambridge, MA, USA, January 2002.
- [35] D. J. C. MacKay. Bayesian methods for backpropagation networks. In E. Domany, J. L. van Hemmen, and K. Schulten, editors, *Models of Neural Networks*, volume 3, chapter 6, pages 211–254. Springer, 1994.
- [36] N. Aronszajn. Theory of reproducing kernels. *Transactions of the American Mathematical Society*, 68:337–404, 1950.

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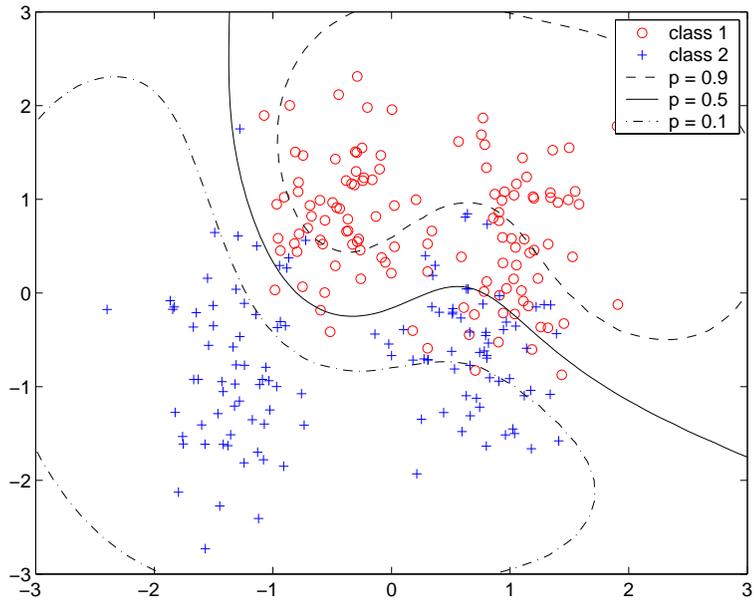


Fig. 1. Output of a Bayesian kernel logistic regression (BKLR) model for Ripley's synthetic benchmark problem [27], the scale parameter of the RBF kernel chosen so as to maximise the marginal likelihood.

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Table 1

Benchmark dataset information, the Pima diabetes dataset is taken from Ripley [27] and is available from <http://www.stats.ox.ac.uk/pub/PRNN>, the remaining benchmarks were from the study by Rätsch [28] and are available from <http://ida.first.gmd.de/~raetsch>.

Benchmark	Training patterns	Test patterns	Input dimension	Realisations
Banana	400	4900	2	100
Breast Cancer	200	77	9	100
Diabetis	468	300	8	100
German	700	300	20	100
Heart	170	100	13	100
Image	1300	1010	18	20
Pima Diabetes	200	332	7	1
Thyroid	140	75	5	100
Titanic	150	2051	3	100
Twonorm	400	7000	20	100
Waveform	400	4600	21	100

Table 2

Cross-entropy and error rate calculated over the test set for kernel logistic regression models with kernel and regularisation parameters determined via the evidence approximation and ten-fold cross-validation for nine benchmark datasets.

Dataset	Cross-Entropy		Error	
	Evidence	Cross-Val	Evidence	Cross-Val
Banana	1168.49±0.36	1180.85±4.46	10.42±0.49	10.48±0.05
Breast Cancer	41.17±0.35	41.50±0.38	26.43±0.48	25.56±0.49
Diabetis	143.59±0.56	145.13±0.83	23.22±0.18	23.56±0.20
Flare Solar	229.38±0.54	229.65±0.66	34.08±0.17	33.88±0.17
Heart	39.65±0.50	40.39±0.50	16.20±0.30	16.85±0.31
Thyroid	9.68±0.45	8.22±0.57	4.89±0.26	4.35±0.23
Titanic	1057.70±3.00	1090.26±8.39	22.63±0.13	22.46±0.09
Twonorm	533.82±4.85	554.12±4.45	2.86±0.03	2.88±0.03
Waveform	1057.21±2.93	1034.84±3.63	10.01±0.04	9.89±0.04

Table 3

Model selection time and number of representers for kernel logistic regression models with kernel and regularisation parameters determined via the evidence approximation and ten-fold cross-validation for nine benchmark datasets.

Dataset	Time in seconds		Representers	
	Evidence	Cross-Val	Evidence	Cross-Val
Banana	64.06±1.76	643.94±17.46	112.84±0.23	118.96±3.84
Breast Cancer	68.13±0.86	307.95±4.43	185.27±0.33	178.57±2.86
Diabetis	564.49±5.36	2418.11±19.38	444.79±1.72	451.65±4.43
Flare Solar	41.98±0.38	454.56±7.76	82.75±0.70	53.40±2.17
Heart	77.41±0.44	219.16±3.43	168.78±0.12	128.44±4.49
Thyroid	23.62±0.21	144.31±1.07	86.6±0.38	115.86±1.73
Titanic	2.84±0.03	38.05±0.35	11.12±0.11	10.78±0.15
Twonorm	1426.35±2.66	2513.31±19.38	388.87±0.59	354.73±7.58
Waveform	1452.05±3.63	2495.55±13.62	400.00±0.00	400.00±0.00

Table 4

Comparison of sparse Bayesian kernel logistic regression, the support vector machine (SVM) and the relevance vector machine (RVM) over seven benchmark datasets, in terms of test set error and the number of representer vectors used. The results for the SVM and RVM are taken from Tipping [14].

Benchmark	Errors			Vectors		
	SVM	RVM	BKLR	SVM	RVM	BKLR
Pima Diabetes	21.1%	19.6%	21.1%	109.0	4.0	14.0
Banana	10.9%	10.8%	10.9%	135.2	11.4	20.9
Breast Cancer	26.9%	29.9%	27.7%	116.7	6.3	5.5
Titanic	22.1%	23.0%	22.6%	93.7	65.3	7.9
Waveform	10.3%	10.9%	10.2%	146.4	14.6	44.3
German	22.6%	22.2%	22.7%	411.2	12.5	189.3
Image	3.0%	3.9%	4.2%	116.6	34.6	694.0