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# Technical Appendix on Sparse Bayesian Regression

Loïc Le Folgoc<sup>1</sup>, Hervé Delingette<sup>1</sup>, Antonio Criminisi<sup>2</sup>, and Nicholas Ayache<sup>1</sup>

<sup>1</sup> Asclepios Research Project, INRIA Sophia Antipolis, France

<sup>2</sup> Machine Learning and Perception Group, Microsoft Research Cambridge, UK

**Abstract.** We report the technical details for a sparse bayesian approach to regression. It can be seen as an extension of the Relevance Vector Machine of Tipping *et al* [1] to a more general setting that can handle vector-valued regression and generic quadratic priors.

## 1 Quadratic Energies & Marginal Likelihood of the Data

We want to minimize in  $\mathbf{w}$  the following cost:

$$E(\mathbf{w}) = (\mathbf{t} - \Phi\mathbf{w})^\top \beta \mathbf{H} (\mathbf{t} - \Phi\mathbf{w}) + \mathbf{w}^\top (\mathbf{A} + \lambda \mathbf{R}) \mathbf{w} \quad (1)$$

and jointly optimize in  $\mathbf{A} = \text{diag}(\mathbf{A}_i)$ ,  $\beta$ ,  $\lambda$ .  $\mathbf{w}|\mathbf{t}, \mathbf{A}, \lambda, \beta$  follows a Gaussian distribution  $\mathcal{N}(\boldsymbol{\mu}, \Sigma)$ , where

$$\boldsymbol{\mu} = \Sigma \Phi^\top \beta \mathbf{H} \mathbf{t}, \quad \Sigma = (\mathbf{A} + \lambda \mathbf{R} + \Phi^\top \beta \mathbf{H} \Phi)^{-1} \quad (2)$$

A key element is that the distribution of  $\mathbf{t}|\mathbf{A}$  is also Gaussian,  $\mathbf{t}|\mathbf{A} \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$ , with

$$\mathbf{C} = (\beta \mathbf{H})^{-1} + \Phi (\mathbf{A} + \lambda \mathbf{R})^{-1} \Phi^\top \quad (3)$$

Indeed, we see that:

$$\begin{aligned} p(\mathbf{t}|\mathbf{A}) &= \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w}|\mathbf{A})d\mathbf{w} \\ &\propto \int \exp -\frac{1}{2}(\mathbf{t} - \Phi\mathbf{w})^\top \beta \mathbf{H} (\mathbf{t} - \Phi\mathbf{w}) \cdot \exp -\frac{1}{2}\mathbf{w}^\top (\mathbf{A} + \lambda \mathbf{R}) \mathbf{w} \cdot d\mathbf{w} \\ &\propto \exp -\frac{1}{2}\boldsymbol{\mu}^\top \Sigma^{-1} \boldsymbol{\mu} \cdot \exp -\frac{1}{2}\mathbf{t}^\top \beta \mathbf{H} \mathbf{t} \cdot \int \exp -\frac{1}{2}(\mathbf{w} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{w} - \boldsymbol{\mu}) d\mathbf{w} \end{aligned}$$

where the integral sums to 1. Thus using (2),

$$p(\mathbf{t}|\mathbf{A}) \propto \exp -\frac{1}{2}\mathbf{t}^\top (\beta \mathbf{H}) \mathbf{t} - \frac{1}{2}\mathbf{t}^\top (\beta \mathbf{H}) \Phi \Sigma \Phi^\top (\beta \mathbf{H}) \mathbf{t}$$

$\mathbf{t}|\mathbf{A}$  is Gaussian since the distribution is proportional to a Gaussian, and by identification it ensues that  $\mathbf{C}^{-1} = \beta \mathbf{H} - (\beta \mathbf{H}) \Phi \Sigma \Phi^\top (\beta \mathbf{H})$ . We then get the desired result using a matrix inversion identity. The fast RVM algorithm proceeds by iteratively implementing a single change to one of the  $\mathbf{A}_i$ 's on the block-diagonal matrix  $\mathbf{A}$ ; specifically the one that maximizes the increase of a quantity known as the *evidence*,  $\log p(\mathbf{t}|\mathbf{A})$ , then re-estimating the parameters of the conditional posterior  $\mathbf{w}|\mathbf{t}, \mathbf{A}, \lambda, \beta$  using (2). The algorithm starts with all  $\mathbf{A}_i$  set to  $\infty$ . The computations involve rank-one "block" updates; it also turns out that the optimal  $\mathbf{A}_i$ 's are rank one matrices (so we actually have rank-one updates).

## 2 Computation of the gain in evidence for a given action

We want to evaluate the change in  $\log p(\mathbf{t}|\mathbf{A}_{-i}, \mathbf{A}_i)$  when a single prior weight  $\mathbf{A}_i$  is changed. Recall that  $\mathbf{t}|\mathbf{A}_{-i}, \mathbf{A}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$ , thus

$$\log p(\mathbf{t}|\mathbf{A}_{-i}, \mathbf{A}_i) = -1/2 \{ \log |\mathbf{C}| + \mathbf{t}^\top \mathbf{C}^{-1} \mathbf{t} \} \quad (4)$$

Now let's single out the contribution of  $\mathbf{A}_i$ , for each of the two terms above. Noting the form of eq. (3), let  $\mathbf{L} = (\mathbf{A} + \lambda \mathbf{R})^{-1}$ . We can single out the contribution of the  $i$ th basis to  $\mathbf{L}$  first, as a rank one update:

$$\mathbf{L} = \begin{pmatrix} \mathbf{L}_{-i} & 0 \\ 0 & 0 \end{pmatrix} + \mathbf{U}_i l_i \mathbf{U}_i^\top \quad (5)$$

with  $\mathbf{U}_i^\top = ((\lambda \mathbf{L}_{-i} \mathbf{R}_i)^\top \mathbf{I}^\top)$  and  $l_i = \{\mathbf{A}_i + \lambda \mathbf{R}_{ii} - (\lambda \mathbf{R}_i)^\top \mathbf{L}_{-i} (\lambda \mathbf{R}_i)\}^{-1} \triangleq \{\mathbf{A}_i + \kappa_i\}^{-1}$ . Note also that any basis for which  $\mathbf{A}_j = \infty$  can be disregarded, since its corresponding line and column in  $\mathbf{L}$  and  $\mathbf{L}_{-i}$  will be null. We can interpret  $\mathbf{L}$  as a square matrix of dimension the number of active bases (including the basis under consideration), and the algorithmic complexity of matrix operations involving  $\mathbf{L}$  or  $\mathbf{L}_{-i}$  will indeed be related to the reduced sized of these matrices. This is also true for  $\mathbf{U}_i$ , as a direct consequence, and for all of the other quantities involved.

Injecting (5) into (3) gives a decomposition of  $\mathbf{C}$  into the sum of a term that does not depend on the  $i$ th basis and of a rank-one term:

$$\mathbf{C} = \mathbf{C}_{-i} + \Phi^i \mathbf{U}_i l_i \mathbf{U}_i^\top \Phi^{i\top} \quad (6)$$

$\Phi$  is superscripted with  $i$  to recall that along with all the other active bases, the  $i$ th basis  $\phi_i$  is present in this matrix. Using rank-one updates for, respectively, the determinant and the inverse, and letting  $\mathbf{C}_{-i}^{-1} \triangleq (\mathbf{C}_{-i})^{-1}$ , we get the two following expressions:

$$|\mathbf{C}| = |\mathbf{C}_{-i}| |l_i| |l_i^{-1} + \mathbf{U}_i^\top \Phi^{i\top} \mathbf{C}_{-i}^{-1} \Phi^i \mathbf{U}_i| \quad (7)$$

$$\mathbf{t}^\top \mathbf{C}^{-1} \mathbf{t} = \mathbf{t}^\top \left( \mathbf{C}_{-i}^{-1} - \mathbf{C}_{-i}^{-1} \Phi^i \mathbf{U}_i \left\{ l_i^{-1} + \mathbf{U}_i^\top \Phi^{i\top} \mathbf{C}_{-i}^{-1} \Phi^i \mathbf{U}_i \right\}^{-1} \mathbf{U}_i^\top \Phi^{i\top} \mathbf{C}_{-i}^{-1} \right) \mathbf{t} \quad (8)$$

These quantities rewrite more compactly if we introduce appropriate notations. Namely, let  $q_j(i) \triangleq \phi_j^\top \mathbf{C}_{-i}^{-1} \mathbf{t} \in \mathbb{R}^d$  and  $s_{jk}(i) \triangleq \phi_j^\top \mathbf{C}_{-i}^{-1} \phi_k \in \mathcal{M}_{d,d}$ . The concatenation of these  $q_j$ 's for all active bases plus the basis under scrutiny (total of  $m$  bases), a.k.a  $\mathbf{q}_i \in \mathbb{R}^{d \times m}$ , will come in helpful. Similarly  $\mathbf{s}_i \in \mathcal{M}_{d \times m, d \times m}$  will denote the matrix with  $s_{kl}(i)$  as  $(k, l)$ th coefficient, where indices span the set of active bases plus the  $i$ th basis. Now, let  $q^i \triangleq \mathbf{U}_i^\top \Phi^{i\top} \mathbf{C}_{-i}^{-1} \mathbf{t} = \mathbf{U}_i^\top \mathbf{q}_i \in \mathbb{R}^d$ , and  $s^i \triangleq \mathbf{U}_i^\top \Phi^{i\top} \mathbf{C}_{-i}^{-1} \Phi^i \mathbf{U}_i = \mathbf{U}_i^\top \mathbf{s}_i \mathbf{U}_i \in \mathcal{M}_{d,d}$ . With these notations in hand and recalling that  $l_i^{-1} = \mathbf{A}_i + \kappa_i$ , we can rewrite eq. (7) and eq. (8) as:

$$\log |\mathbf{C}| = \log |\mathbf{C}_{-i}| - \log |\mathbf{A}_i + \kappa_i| + \log |\mathbf{A}_i + \kappa_i + s^i| \quad (9)$$

$$\mathbf{t}^\top \mathbf{C}^{-1} \mathbf{t} = \mathbf{t}^\top \mathbf{C}_{-i}^{-1} \mathbf{t} - q^{i\top} \{ \mathbf{A}_i + \kappa_i + s^i \}^{-1} q^i \quad (10)$$

Ignoring the terms that do not depend on the  $i$ th basis, we see that the contribution to the evidence of the model for a given value of  $\mathbf{A}_i$  is directly related to:

$$l(\mathbf{A}_i) = \log |\mathbf{A}_i + \kappa_i| - \log |\mathbf{A}_i + \kappa_i + s^i| + q^{i\top} \{\mathbf{A}_i + \kappa_i + s^i\}^{-1} q^i \quad (11)$$

Naturally if  $\lambda = 0$  (no additional regularization) this comes down to the regular RVM, with  $q^i = q_i$ ,  $s^i = s_{ii}$  and  $\kappa_i = 0$ .

### 3 Maximization of the gain in evidence

If  $q^i q^{i\top} - s^i$  has no positive eigenvalue, the maximum  $\mathbf{A}_i$  lies at infinity and the basis should remain inactive, or be removed. Otherwise the gradient of Eq. (11) provides ground to look for rank-one maximizers  $\mathbf{A}_i = \alpha_i \eta_i \eta_i^\top$ . To that aim we compute  $n_i = s^{i-1} q^i$  and

$$a_i = \frac{(n_i^\top s^i n_i)^2}{(n_i^\top q^i)^2 - n_i^\top s^i n_i} - n_i^\top \kappa_i n_i \quad (12)$$

If  $a_i \geq 0$  the maximizer is given by  $\alpha_i = a_i$  and  $\eta_i = n_i$ . Otherwise ( $a_i < 0$ ) we set  $\alpha_i = 0$  and numerically solve over the optimal orientation  $\eta_i$ . This latter case arises when the regularization level alone is sufficient to make additional "shrinkage" unnecessary.

### 4 Update of $\lambda$

We derive an update rule via an expectation-maximization procedure. Knowing  $\mathbf{w}$ , it would be straightforward to derive an estimate of  $\lambda$  by maximizing the log-likelihood of  $\mathbf{w}$  or the posterior of  $\lambda$  given  $\mathbf{w}$ . However  $\mathbf{w}$  is hidden in our model. Instead, we try to maximize the log-likelihood on average (i.e. to minimize the average loss):  $\max_{\lambda} \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})} [\log p(\mathbf{t}, \mathbf{w} | \mathbf{A}, \lambda, \beta) | \mathbf{A}^*, \beta^*]$ , where  $\mathbf{A}^*$  and  $\beta^*$  are our current estimates of the respective quantities. Discarding terms which are constants of  $\lambda$ , we obtain the following:

$$\lambda^* = \arg \max_{\lambda} -\frac{\lambda}{2} \text{tr}(\boldsymbol{\Sigma} \mathbf{R}) + \frac{1}{2} \log |\mathbf{A} + \lambda \mathbf{R}| - \frac{\lambda}{2} \boldsymbol{\mu}^\top \mathbf{R} \boldsymbol{\mu} \quad (13)$$

Deriving leads to:

$$\frac{\partial}{\partial \lambda} f(\lambda) \propto \text{tr}(\{\mathbf{A} + \lambda \mathbf{R}\}^{-1} \mathbf{R}) - \text{tr}(\boldsymbol{\Sigma} \mathbf{R}) - \boldsymbol{\mu}^\top \mathbf{R} \boldsymbol{\mu} \quad (14)$$

This is a decreasing function of  $\lambda$  and thus has at most one zero. If  $\frac{\partial}{\partial \lambda} f(\lambda)$  is negative at the origin,  $\lambda^* = 0$ . Otherwise, we optimize by using the Newton method on a log scale. This is motivated by the fact that the function of interest is not only decreasing, but also smooth and convex. Lastly note that  $\{\mathbf{A} + \lambda \mathbf{R}\}^{-1} \mathbf{R} = \{\mathbf{R}^{-1} \mathbf{A} + \lambda \mathbf{I}\}^{-1}$ , so we can compute the eigenvalues  $\delta_k$  of  $\mathbf{A}^{1/2} \mathbf{R}^{-1} \mathbf{A}^{1/2}$  once and rely on the fact that  $\text{tr}(\{\mathbf{A} + \lambda \mathbf{R}\}^{-1} \mathbf{R}) = \sum_k 1/(\delta_k + \lambda)$  to avoid repeated matrix inversions.

## References

1. Tipping, M.E., Faul, A.C., et al.: Fast marginal likelihood maximisation for sparse bayesian models. In: Workshop on artificial intelligence and statistics. Volume 1., Jan (2003)