An Integrated Generative and Discriminative Bayesian Model for Binary Classification

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Introduction

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To alleviate this problem, we have developed a statistical model that uses a small number of meta-covariates inferred from the data through a Gaussian mixture model, rather than all the original covariates, to classify samples.
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To alleviate this problem, we have developed a statistical model that uses a small number of meta-covariates inferred from the data through a Gaussian mixture model, rather than all the original covariates, to classify samples.

The novelty of our approach is that our meta-covariates are formed considering predictor-outcome correlations as well as inter-predictor correlations.
This idea was partly inspired by recent empirical research that has shown that optimum predictive performance often corresponds to an intermediate trade-off between the purely generative and purely discriminative approaches to classification.
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The main advantage over using a sparse classification model is that we can extract a much larger subset of covariates with essential predictive power and partition this subset into groups, within which the covariates are similar.

Moreover, our meta-covariates have a natural ordering and interpretation as increasingly predictive response-relevant clusters.
Here, the meta-covariate method is applied to gene expression data. Co-expression clusters are identified and represented by its mean. Each cluster mean is assigned a weight according to its ability to distinguish between set A and set B data.
Model notation

\( \mathbf{X} \) Design matrix
\( \mathbf{t} \) Response vector
\( \mathbf{\theta} \) Matrix of clustering mean parameters \( \theta_{kn} \)
\( \mathbf{\Sigma} \) Matrix of clustering variance parameters
\( \mathbf{\pi} \) Vector of mixing coefficients
\( \mathbf{Z} \) Matrix of clustering latent variables
\( w_0 \) Regression bias parameter
\( \mathbf{w} \) Vector of regression coefficients
\( \mathbf{y} \) Vector of classification auxiliary variables

\( N \times D \quad \mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_D] \)
\( N \times 1 \quad t_n \in \{0, 1\} \)
\( K \times N \quad K \text{ meta-covariates } \theta_k \)
\( K \times N \quad \sigma^2_{kn} \)
\( K \times 1 \quad \pi_k \)
\( D \times K \quad z_{dk} \in \{0, 1\} \)
\( 1 \times 1 \quad \text{Scalar intercept} \)
\( K \times 1 \quad w_k \)
\( N \times 1 \quad y_n \)
Joint distribution:

\[ p(t, y, X, Z, \pi, \theta, \Sigma, w_0, w) = p(t, y | \theta, w_0, w) \cdot p(X, Z | \pi, \theta, \Sigma) \cdot p(\pi) \cdot p(\theta | \Sigma) \cdot p(\Sigma) \cdot p(w_0) \cdot p(w). \]
Joint distribution:

\[ p(t, y, X, Z, \pi, \theta, \Sigma, w_0, w) = p(t, y|\theta, w_0, w) p(X, Z|\pi, \theta, \Sigma) p(\pi) p(\theta|\Sigma) p(\Sigma) p(w_0) p(w). \]
Model components

Generative component:

\[
p(X, Z | \pi, \theta, \Sigma) = \prod_{d=1}^{D} \prod_{k=1}^{K} \pi_k^{Z_{dk}} \mathcal{N}(x_d | \theta_k, \Sigma_k)^{z_{dk}}, \text{ where } \Sigma_k = \text{diag}(\sigma_{k1}^2, \ldots, \sigma_{kN}^2).
\]
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Discriminative component:

\[ p(t, y | \theta, w_0, w) = \prod_{n=1}^{N} p(t_n | y_n)p(y_n | \theta_n, w_0, w), \text{ where } \]

\[ p(t_n | y_n) = \begin{cases} \delta(y_n > 0) & \text{if } t_n = 1 \\ \delta(y_n \leq 0) & \text{otherwise} \end{cases} \]

and \( p(y_n | \theta_n, w_0, w) = \mathcal{N}(y_n | w_0 + w^T \theta_n, 1). \)
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\[
\text{and } p(y_n|\theta_n, w_0, w) = \mathcal{N}(y_n|w_0 + w^T \theta_n, 1).
\]

Prior distributions:

\[
p(\pi) = \text{const}, \quad p(\theta|\Sigma) = \prod_{k=1}^{K} \mathcal{N}(\theta_k|\theta_0, h\Sigma_k),
\]

\[
p(\Sigma) = \prod_{k=1}^{K} \prod_{n=1}^{N} \text{Inv-Gamma} \left( \sigma_{kn}^2 \bigg| \nu, \xi \right), \quad p(w_0) = \mathcal{N}(w_0|0, l_0) \text{ and } p(w) = \mathcal{N}(w|0, ll).\]
EM algorithm: the E-step

\[
\gamma(Z_{dk}) = \frac{\pi_k \left( \prod_n \sigma_{kn}^2 \right)^{-1/2} \exp \left\{ -\frac{1}{2} \sum_n \frac{(x_{nd} - \theta_{kn})^2}{\sigma_{kn}^2} \right\}}{\sum_j \pi_j \left( \prod_n \sigma_{jn}^2 \right)^{-1/2} \exp \left\{ -\frac{1}{2} \sum_n \frac{(x_{nd} - \theta_{jn})^2}{\sigma_{jn}^2} \right\}},
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Keith Harris (University of Glasgow)  Generative and Discriminative Bayesian Model  October 16th 2010  8 / 20
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\]

\[
E(y_n) = \begin{cases} 
    w_0 + w^T \theta_n + \frac{\phi(-w_0 - w^T \theta_n)}{1 - \Phi(-w_0 - w^T \theta_n)} & \text{if } t_n = 1 \\
    w_0 + w^T \theta_n - \frac{\phi(-w_0 - w^T \theta_n)}{\Phi(-w_0 - w^T \theta_n)} & \text{otherwise}.
\end{cases}
\]
EM algorithm: the M-step

\[
\theta_{kn} = \frac{ \left( E(y_n) - w_0 - \sum_{k' \neq k} w_{k'} \theta_{k'n} \right) w_k + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} \gamma(Z_{dk}) x_{nd} + \frac{\theta_{0n}}{h} \right) }{ w_k^2 + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} \gamma(Z_{dk}) + \frac{1}{h} \right) },
\]

Note that the first component of \( w \) is set to 1, so that the model is identifiable.
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\]

\[
w_k^2 + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} \gamma(z_{dk}) + \frac{1}{h} \right)
\]

\[
\sigma_{kn}^2 = \frac{\sum_{d=1}^{D} \gamma(z_{dk})(x_{nd} - \theta_{kn})^2 + \frac{1}{h}(\theta_{kn} - \theta_{0n})^2 + 2\xi}{\sum_{d=1}^{D} \gamma(z_{dk}) + 2\nu + 3}
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\[ \theta_{kn} = \left( \frac{E(y_n) - w_0 - \sum_{k' \neq k} w_{k' \theta_k n}}{w_h^2 + \frac{\sigma^2_{kn}}{\sigma^2_{kn}}} \left( \sum_{d=1}^D \gamma(Z_{dk}) x_{nd} + \frac{\theta_{0n}}{h} \right) \right) \]

\[ \sigma^2_{kn} = \frac{\sum_{d=1}^D \gamma(Z_{dk})(x_{nd} - \theta_{kn})^2 + \frac{1}{h}(\theta_{kn} - \theta_{0n})^2 + 2\xi}{\sum_{d=1}^D \gamma(Z_{dk}) + 2\nu + 3} \]

\[ \pi_k = \frac{1}{D} \sum_{d=1}^D \gamma(Z_{dk}), \]
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\[
\theta_{kn} = \left( E(y_n) - w_0 - \sum_{k' \neq k} w_{k'} \theta_{k'n} \right) \frac{w_k}{w_k^2 + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} \gamma(Z_{dk}) x_{nd} + \frac{\theta_{0n}}{h} \right)} \frac{\sum_{d=1}^{D} \gamma(Z_{dk}) (x_{nd} - \theta_{kn})^2 + \frac{1}{h} (\theta_{kn} - \theta_{0n})^2 + 2 \xi}{\sum_{d=1}^{D} \gamma(Z_{dk}) + 2 \nu + 3},
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\[
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\[
w_0 = \frac{\sum_{n=1}^{N} \left( E(y_n) - \sum_{k'=1}^{K} w_{k'} \theta_{k'n} \right)}{N + \frac{1}{l_0}},
\]
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\theta_{kn} = \frac{\left( E(y_n) - w_0 - \sum_{k' \neq k} w_{k'} \theta_{k' n} \right) w_k + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} \gamma(Z_{dk}) x_{nd} + \frac{\theta_{0n}}{h} \right)}{w_k^2 + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} \gamma(Z_{dk}) + \frac{1}{h} \right)},
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\[
w = \left( \theta \theta^T + \frac{1}{l} \right)^{-1} \theta (E(y) - w_0 1).
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$$w = \left( \theta \theta^T + \frac{1}{l}I \right)^{-1} \theta \left( E(y) - w_0 1 \right).$$

Note that the first component of $w$ is set to 1, so that the model is identifiable.
Hypertension is a common precursor to cardiovascular disease and is often exacerbated by increased dietary intake of sodium.
Insights into salt-sensitive hypertension

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By analysing microarray data of the SP, a salt-insensitive strain (WKY) and an intermediate congenic strain (2a), the genes and pathways that influence salt-sensitive hypertension can be elucidated.
Characterising cluster 13 of the meta-covariate model with $K = 20$ clusters suggested by BIC. The expression of all 13 genes (left top); the mean expression (left middle) and alternative $\theta$ (meta-covariate) representation (left bottom).
RP analysis of this cluster

The genes in cluster 13, overlaid with 2a (left top), WKY (right top) and SP (left bottom) rank products results: red indicates over-expression on salt, while green indicates under-expression on salt.
Circadian rhythm genes are implicated

Canonical pathway analysis of cluster 13 shows that this cluster is enriched for circadian rhythm genes, implicating circadian rhythm genes as important in differentiating between salt-loaded and non salt-loaded animals.

This is relevant, given that these nocturnal animals exhibit increased hypertension during the night, and this difference is exacerbated on salt-loading.

Now we consider how these genes are related to the strains. We saw from the RP analysis of cluster 13 that there are differences on salt-loading in the 2a and WKY strains, but not in the SP strain.

We can therefore hypothesize that the genes in the most influential meta-covariate cluster are protective against hypertension in response to an increase in dietary sodium.
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Extension to Gibbs sampling

The full conditional distribution for $\pi$:

$$\text{Dirichlet}\left(\sum_{d=1}^{D} z_{d1} + 1, \ldots, \sum_{d=1}^{D} z_{dK} + 1\right).$$
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The full conditional distribution for $\theta_{kn}$:

$$\mathcal{N}((e_n w_k + m_{kn}) v_{kn}, v_{kn}), \text{ where } e_n = y_n - w_0 - \sum_{k' \neq k} w_{k'}, \theta_{k'n},$$

$$m_{kn} = \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} z_{dk} x_{nd} + \frac{\theta_{0n}}{h} \right) \text{ and } v_{kn} = \left[ w_{k}^2 + \frac{1}{\sigma_{kn}^2} \left( \sum_{d=1}^{D} z_{dk} + \frac{1}{h} \right) \right]^{-1}.$$
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The full conditional distribution for $\sigma_{kn}^2$:

$$\text{Inv-Gamma} \left( \frac{1}{2} \sum_{d=1}^{D} z_{dk} + \nu + \frac{1}{2}, \frac{1}{2} \sum_{d=1}^{D} z_{dk} (x_{nd} - \theta_{kn})^2 + \frac{1}{2h} (\theta_{kn} - \theta_{0n})^2 + \xi \right).$$
Extension to Gibbs sampling continued

The full conditional distribution for $w_0$:

$$\mathcal{N}\left(\frac{\sum_{n=1}^{N} \left( y_n - \sum_{k'=1}^{K} w_{k'} \theta_{k'n} \right)}{N + \frac{1}{l_0}}, \left( N + \frac{1}{l_0} \right)^{-1} \right).$$
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The full conditional distribution for $w$:

$$\mathcal{N}\left(\left(\theta \theta^T + \frac{1}{l} I\right)^{-1} \theta (y - w_0 1), \left(\theta \theta^T + \frac{1}{l} I\right)^{-1}\right).$$
Extension to Gibbs sampling continued

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$$
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$$

The full conditional distribution for $z_d$: Multinomial($n_{\text{trials}}, p_1, \ldots, p_K$), where $n_{\text{trials}} = 1$ and $p_k = \gamma(z_{dk})$. 
Extension to Gibbs sampling continued

The full conditional distribution for $w_0$:

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The full conditional distribution for $y_n$:

$$
p(y_n|y_{-n}, \pi, \theta, \Sigma, w_0, w, t, X, Z) \propto \begin{cases} 
\delta(y_n > 0) \mathcal{N}(y_n|w_0 + w^T \theta_n, 1) & \text{if } t_n = 1 \\
\delta(y_n \leq 0) \mathcal{N}(y_n|w_0 + w^T \theta_n, 1) & \text{otherwise.}
\end{cases}
$$
Posterior predictive distribution

We obtain the predictive classification of a new observation $t^*$, conditioning on the test point $x^*$, using the Monte-Carlo estimate:

$$P(t^* = 1|x^*, t, X) \approx \frac{1}{m} \sum_{t=1}^{m} \Phi \left( w_0^{(t)} + w^{(t)} \theta^{*(t)} \right),$$

where $w_0^{(t)}$, $w^{(t)}$ and $\theta^{*(t)}$ are the MCMC samples of the parameters $w_0$, $w$ and $\theta^*$. 
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where $w_0^{(t)}$, $w^{(t)}$ and $\theta^{*}(t)$ are the MCMC samples of the parameters $w_0$, $w$ and $\theta^*$.

Thus, we also need to sample $\theta_k^*$ from:

$$\mathcal{N} \left( \frac{\sum_{d=1}^{D} Z_{dk} x_d^* + \theta_0^*}{\sum_{d=1}^{D} Z_{dk} + \frac{1}{h}}, \left[ \frac{1}{\sigma_k^{*2}} \left( \sum_{d=1}^{D} Z_{dk} + \frac{1}{h} \right) \right]^{-1} \right),$$

and $\sigma_k^{*2}$ from:

$$\text{Inv-Gamma} \left( \frac{1}{2} \sum_{d=1}^{D} Z_{dk} + \nu + \frac{1}{2}, \frac{1}{2} \sum_{d=1}^{D} Z_{dk} (x_d^* - \theta_k^*)^2 + \frac{1}{2} (\theta_k^* - \theta_0^*)^2 + \xi \right).$$
Hedenfalk’s breast cancer data

We apply our method to a publicly available breast cancer dataset from patients carrying mutations in the predisposing genes, BRCA1 or BRCA2, and from patients not expected to carry either of these hereditary predisposing mutations.

\[ D = 3226, \quad N = 22 \] (7 BRCA1, 8 BRCA2 and 7 sporadic).

A Wilcoxon rank-sum test was used to provide a ranking of the features based on their p-value. Setting a threshold of 10% the number of features was reduced to 626.
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We use our method to classify BRCA1 versus the others and compare our method to a Bayesian sparse probit regression model.

We initialised our Gibbs sampler using the EM algorithm.

We ran the Gibbs samplers of both methods for 100000 iterations and discard the first half of each chain as burn-in.

We compared the methods using leave-one-out cross validation.
Plots of the posterior predictive probabilities

**Posterior Predictive Probabilities from our Meta–Covariate Model**

**Posterior Predictive Probabilities from Sparse Probit Regression**
Our experimental results thus indicate that our Gibbs sampling approach of inferring meta-covariates in classification has competitive performance with Bayesian sparse probit regression.

Moreover, our approach can be naturally extended to multiclass classification. Future research will focus on applying our methodology to functional magnetic resonance imaging data and developing a Bayesian sampler that can infer directly from the data the optimal number of clusters in our model via an infinite mixture model.
Conclusions

Our experimental results thus indicate that our Gibbs sampling approach of inferring meta-covariates in classification has competitive performance with Bayesian sparse probit regression.

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