A nested expectation–maximization algorithm for latent class models with covariates

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Abstract
We propose a novel nested expectation–maximization algorithm for latent class models with covariates which allows maximization of the full–model log-likelihood and, differently from current methods, is characterized by a monotone log-likelihood sequence.

Keywords: \em algorithm, Latent class model, Multivariate categorical data, Pólya-gamma

1. Introduction
Multivariate categorical data are routinely collected in several fields of research [e.g. 15]. In these settings, it is of key interest to characterize the dependence structures in the observed data, and to identify the underlying classes or subpopulations which may explain these patterns of dependence, and their changes with external covariates. Let $Y_i = (Y_{i1}, \ldots, Y_{iJ})^\top$, denote the multivariate categorical random variable generating the observed data $y_i = (y_{i1}, \ldots, y_{iJ})^\top \in \mathcal{Y} = \{1, \ldots, K_1\} \times \cdots \times \{1, \ldots, K_J\}$, for every unit $i = 1, \ldots, n$. Latent class models with covariates \cite{3, 9, 11} address this goal by assuming the response variables $Y_{i1}, \ldots, Y_{iJ}$, are conditionally independent given a latent class indicator $s_i \in S = \{1, \ldots, R\}$, whose probability mass function is allowed to change with the covariates $X_i = (x_{i1}, \ldots, x_{iP})^\top \in \mathcal{X}$, under a multinomial logistic regression. Consistent with this, the conditional probability mass function $p(Y_{ij} = y_{ij} | X_i)$ can be expressed as a covariate–dependent mixture of products of multinomial distributions, providing

$$p(Y_j = y | X_i) = \sum_{r=1}^{R} v_r(x_i) \prod_{j=1}^{J} \pi_{jr}(y_j) = \sum_{r=1}^{R} \frac{\exp(X_i^\top \beta_r)}{\sum_{j=1}^{J} \exp(X_i^\top \beta_j)} \prod_{j=1}^{J} \pi_{jr}(y_j), \quad \text{for each } i = 1, \ldots, n, \quad (1)$$

where $v_r(x_i) = p(s_i = r | X_i) \in (0, 1)$ is the covariate–dependent probability of the class $r$, whereas $\pi_{jr}(y_j) = p(Y_{ij} = y_{ij} | s_i = r) \in (0, 1)$ characterizes the probability to observe the category $y_j$ for the variable $Y_{ij}$ in class $r$. Note also that, consistent with classical multinomial logistic regression, the coefficients vector $\beta_R = (\beta_{1R}, \ldots, \beta_{PR})^\top$ associated with the last class $R$ is fixed to zero, in order to avoid identifiability issues. With this choice, $X_i^\top \beta_r$ measures the log-odds of belonging to class $r$ instead of class $R$, when the vector of covariates is $X_i$. Equation (1) provides an interpretable factorization for the joint probability mass function of the categorical random vector $Y_i = (Y_{i1}, \ldots, Y_{iJ})^\top$, which allows inference on the class-specific generative mechanisms underlying the observed data $y_i$, and how the latent classes $s_i$ relate to the covariates $X_i$. Refer to \cite{3, 9, 11} for a discussion about this class of models, and to \cite{8} for a review on latent class analysis, including seminal contributions which rely on representations without covariates \cite{13, 18, 20}.

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To obtain the above information, it is necessary to estimate $\beta = [\beta_1, \ldots, \beta_{K-1}]$ and $\pi = [\pi_j(y_i), \ldots, \pi_j(y_J): j = 1, \ldots, J; y_j = 1, \ldots, K_j]$. This can be accomplished by maximizing the log-likelihood function

$$\ell(\beta, \pi; y, x) = \sum_{i=1}^{n} \log \left( \sum_{r=1}^{R} \pi_r(y_i) \prod_{j=1}^{K_i} \pi_j(y_i)^{1(y_{ij} = y_j)} \right) = \sum_{i=1}^{n} \log \left( \sum_{r=1}^{R} \frac{\exp(x_i^\top \beta_r)}{\sum_{l=1}^{R} \exp(x_i^\top \beta_l)} \prod_{j=1}^{K_i} \pi_j(y_i)^{1(y_{ij} = y_j)} \right). \quad (2)$$

where $1(y_{ij} = y_j) = 1$ if $y_{ij} = y_j$, and 0 otherwise. However, direct maximization of $\ell(\beta, \pi; y, x)$ is not straightforward due to the sum inside the logarithm. In fact, although a subset of contributions attempt direct maximization of (2) via Newton–Rapshon [27, 14] or Simplex algorithms [9], more popular implementations [3, 11, 24, 6, 25] rely instead on EM routines [13], leveraging a hierarchical specification—equivalent to (1)—which introduces a latent class variable $s_i \in \mathcal{S} = \{1, \ldots, R\}$ for each unit $i = 1, \ldots, n$, to obtain the generative process

$$(Y_{ij} | s_i = r) \sim \text{categorical}(\pi_{jr}, K_j), \text{ for any } j = 1, \ldots, J, \quad (s_i | x_i) \sim \text{categorical}(\nu(x_i), R),$$

(3)

independently for each $i = 1, \ldots, n$. In (3), categorical($\rho, H$) denotes the generic categorical random variable having probability mass function $\rho = [\rho_1, \ldots, \rho_H]$ for the $H$ different categories. Hence, consistent with (3), if $s_1, \ldots, s_n$ are known, the maximum likelihood estimates for $\beta$ and $\pi$ can be easily obtained by maximizing separately the log-likelihood $\ell_1(\beta; s, x)$ associated with the multinomial logistic regression for $s_1, \ldots, s_n$, and the log-likelihood $\ell_2(\pi; y, s)$ for the categorical data $y_{1j}, \ldots, y_{nj}, j = 1, \ldots, J$, within each subpopulation defined by the classes $s_1, \ldots, s_n$. In fact

$$\ell_1(\beta; s, x) + \ell_2(\pi; y, s) = \sum_{i=1}^{n} \sum_{r=1}^{R} 1(s_i = r) \log \left[ \frac{\exp(x_i^\top \beta_r)}{\sum_{l=1}^{R} \exp(x_i^\top \beta_l)} \right] + \sum_{i=1}^{n} \sum_{r=1}^{R} \sum_{j=1}^{K_i} 1(s_i = r) 1(y_{ij} = y_j) \log \pi_j(y_j) \quad (4)$$

Specifically, the maximization of $\ell_1(\beta; s, x)$ in equation (4), with respect to $\beta$, requires algorithms for multinomial logistic regressions, within a generalized linear models framework [e.g. 1, Chapter 7], whereas $\ell_2(\pi; y, s)$ is analytically maximized at $\hat{\pi}(y_i) = \frac{[\sum_{r=1}^{R} 1(s_i = r) 1(y_{ij} = y_j)]}{\sum_{r=1}^{R} 1(s_i = r)}$, [e.g. 1, Chapter 1], for every $r = 1, \ldots, R$, $j = 1, \ldots, J$, and $y_j = 1, \ldots, K_j$. Unfortunately, the class memberships $s_1, \ldots, s_n$ are not observed, but characterize latent subpopulations underlying the observed data $y_1, \ldots, y_n$. Therefore, estimation of $\beta$ and $\pi$ needs to rely only on the information provided by the data $(y_i, x_i)$, for $i = 1, \ldots, n$.

There are two main strategies in the literature to estimate $\beta$ and $\pi$, generally referred to as one–step [3, 11, 24], and three–step [6, 25] methods. The former attempt a simultaneous estimation of $\beta$ and $\pi$ in $\ell(\beta, \pi; y, x)$ (2), leveraging the augmented log-likelihood $\ell(\beta, \pi; y, s, x) = \ell_1(\beta; s, x) + \ell_2(\pi; y, s)$ in (4). The latter consider, instead, a multi–step routine which first estimates the latent classes $s_1, \ldots, s_n$, along with $\pi$, from a latent class model without covariates, and then uses these predicted classes as responses in $\ell_1(\beta; s, x)$—or a modification of it—to estimate $\beta$.

Although the above computational methods are routinely considered in standard implementations, including the R library poLCA [19] and the software LATENT GOLD [26], as discussed in Sect. 1.1 and 1.2, both strategies still raise open questions on the quality of the estimates, and on the efficiency of the associated algorithms. Motivated by these issues, Sect. 2 describes a nested EM algorithm we propose to improve inference within this class of models. As carefully highlighted in a real data application in Sect. 3, our novel computational strategy is characterized by improved theoretical properties, and superior estimating performance.
1.1. One-step estimation methods

Recalling the discussion in Sect. 1, maximum likelihood estimation of the parameters in the full statistical model (1)—characterizing one-step methods [3, 11, 24]—proceeds via an EM algorithm which leverages the complete log-likelihood function $\ell(\beta, \pi; y, s, x)$ in (4) for the data $(y_i, x_i)$, and the augmented latent class variable $s_i$, $i = 1, \ldots, n$. In fact, recalling the generative process in equation (3), this complete log-likelihood is simpler than (2), since it can be expressed as the sum of the log-likelihood $\ell_1(\beta; s, x)$ associated with the multinomial logistic regression for $s_1, \ldots, s_n$, and the set of conditionally independent log-likelihoods $\ell_2(\pi; y, s)$ for the categorical data $y_1, \ldots, y_n$, within each subpopulation defined by the classes $s_1, \ldots, s_n$. This result allows separate estimation for the coefficients $\beta$ of the multinomial logistic regression, and for the probabilities $\pi$ of the categorical variables. Moreover, $\ell_1(\beta; s, x)$ and $\ell_2(\pi; y, s)$, are linear in the augmented data $1(s_i = r)$. Letting $\theta = (\beta, \pi)$, this facilitates a simple expectation step in which, at the general iteration $t$, each $1(s_i = r)$ in (4) is replaced with

$$s_{ir}^t = E[1(s_i = r) | \theta^t, y, x_i] = \frac{\exp[x_i^T \beta^t]}{\sum_{r=1}^R \exp[x_i^T \beta^t]} \prod_{j=1}^{K_i} \pi_{jr}^{t-1}(y_j) \sum_{r=1}^R \exp[x_i^T \beta^t] \prod_{j=1}^{K_i} \pi_{jr}^{t-1}(y_j),$$

for each $r = 1, \ldots, R, i = 1, \ldots, n, t \geq 1$.

It is instead not possible to maximize analytically $Q_1(\beta | \theta^t)$ with respect to $\beta$, due to the logistic link. To address this issue [11] and [24] consider one Newton–Raphson step relying on a quadratic approximation of $Q_1(\beta | \theta^t)$. This strategy provides the $m$ updating step $\beta^{t+1} = \beta^t - H_{\beta\beta}^{-1}(\beta^t) V_{\beta\theta}$, with $H_{\beta\beta} \theta^t$ and $V_{\beta\theta}$ denoting the Hessian and the gradient of the expected log-likelihood $Q_1(\beta | \theta^t)$ with respect to $\beta$, evaluated at $\beta^t$. The routine proposed by [3] considers instead a slightly different approach relying on the Hessian and the gradient computed from full–model log-likelihood $\ell(\beta, \pi; y, x)$ in (2), and evaluated at $(\beta^t, \pi^t)$ and $s_{ir}^t$, $r = 1, \ldots, R, i = 1, \ldots, n$. This procedure—currently implemented in R library poLCA [19]—partially breaks the EM rationale, since the step for $\beta$ maximizes a plug–in estimate of a quadratic approximation for $\ell(\beta; y, x)$, instead of $Q_1(\beta | \theta^t)$. Hence, although this approach allows direct estimation of the standard errors during the maximization procedure, it may provide a less stable routine.

Although the above solutions provide a standard approach to obtain $\beta^{t+1}$, the resulting computational routines guarantee neither $Q_1(\beta^{t+1} | \theta^t) \geq Q_1(\beta | \theta^t)$, nor $Q_1(\beta^{t+1} | \theta^t) \geq Q_1(\beta^t | \theta^t)$ [4, 5], and therefore the proposed methodologies are neither an EM algorithm, nor a generalized EM algorithm, respectively [10]. Failure to improve the expected log-likelihood may also affect the monotonicity of the log-likelihood sequence $\ell(\theta^t, \pi^t; y, x)$, thereby providing routines which do not meet the fundamental properties of the EM, and may not guarantee reliable
ELECTION DATA: Two Latent Classes

$0$  $5$  $10$  $15$

$-16000$

$-14000$

$-12000$

iteration

$l(\theta(t); x, y)$

ELECTION DATA: Three Latent Classes

$0$  $5$  $10$  $15$

$-17500$

$-15000$

$-12500$

iteration

$l(\theta(t); x, y)$

Figure 1. Graphical representation of the log-likelihood sequence $l(\beta(t), \pi(t); y, x) = l(\theta(t); x, y)$, $t = 1, \ldots$, produced by the routines discussed in Sect. 1.1: EM algorithm with Newton–Raphson as implemented by [3] (—), EM algorithm with Newton–Raphson as implemented by [11, 24] (- - -), EM algorithm with Newton–Raphson as implemented by [11, 24] with step-size control $\alpha = 0.5$ (---), nested EM algorithm proposed in Sect. 2 (-- -- --), monotone MM algorithm with correction proposed by [4, 5] (•••).

convergence [e.g. 21, Chapter 1.5.5]. As shown in Fig. 1, this absence of monotonicity for the log-likelihood sequence is not just found in pathological scenarios, but arises also in simple routine applications, and may substantially affect convergence to the maximum log-likelihood. Although carefully tuned routines can be designed to overcome these issues, we shall emphasize that the multinomial logit log-likelihood characterizing $Q_{i}(\beta \mid \theta^{(t)})$ is defined on a set of latent responses whose expectation (5) changes at every iteration of the algorithm. This is more problematic compared to classical multinomial logistic regression with observed responses, and is further complicated by the need to estimate $\pi$ along with $\beta$ in (1). Hence, unstable updating steps may have a major effect on the efficiency of the entire algorithm and on the quality of inference, thus requiring finer maximization.

To mitigate the above issues, standard implementations of the one–step approach consider multiple runs of the above EM based on different initializations, and rely on the routine converging to the highest log-likelihood for inference. Alternatively, internal checks can be implemented to control for decays in the log-likelihood sequence, and re-start the routine from different initial values when a decay is found. These strategies reduce concerns about unstable routines, but require multiple runs which increase the computational cost. A possible solution to reduce the chance of a decay in the log-likelihood sequence, without relying on multiple runs, is to rescale $H^{-1}_{i\beta i\beta}V_{i\beta i\beta} = \Lambda^{(t)}$ by a tuning parameter $0 < \alpha \leq 1$, so that $\beta^{(t+1)} = \beta^{(t)} - \alpha \Delta^{(t)}$ [e.g. 21, Chapter 1.5.6]. However, the implementation requires the choice of $\alpha$, without theory on optimal settings. Moreover, there is a trade–off between accuracy and computational efficiency in the choice of $\alpha$. Indeed, when $\alpha$ decreases, the routine is more stable, but convergence is slower.

Motivated by the above issues, [4] and [5] proposed a Minorize–Majorize (MM) algorithm [e.g. 17] for logistic and multinomial logit regression, respectively, which ensures monotonicity in the log-likelihood sequence. Their computational routine replaces the Hessian with a lower–bound matrix $B$ to obtain a quadratic function $g(\beta \mid \beta^{(t)})$ which minorizes the log-likelihood at every $\beta$ and is tangent to it in $\beta^{(t)}$. This provides a simple and tractable updating scheme similar to the Newton–Raphson—with $H^{-1}$ replaced by $B^{-1}$—while additionally guaranteeing monotone
log-likelihood sequences. Although this strategy is currently not implemented in algorithms for latent class models with covariates, we shall notice that the procedures proposed by [4] and [5] can be easily incorporated in the $m$–step for $\beta$ by replacing the observed response data in their routines with the expectation of the latent class variables computed in (5). As shown in Fig. 1, this procedure effectively provides a monotone log-likelihood sequence, but requires more iterations to reach convergence compared to the nested EM algorithm we propose in Sect. 2.

1.2. Three–step estimation methods

Differently from one–step methods, the classical three–step procedures [e.g. 8] do not attempt direct maximization of the log-likelihood (2) for the full model (1), but instead rely on the following multi–step strategy:

1. Estimate the parameters $\pi$ and the class probabilities $\nu = (\nu_1, \ldots, \nu_R)$ from a latent class model without covariates. This requires maximization of $\ell(\nu, \pi; y) = \sum_{i=1}^{n} \log \{ \sum_{r=1}^{R} \nu_r \prod_{j=1}^{K} \pi_{jr}(y_j) \} \pi_1(s_i y) \prod_{j=1}^{K} \pi_{jr}(y_j)^{(s_i y)_j}, \nu \leq 1, \ldots, R$. Note that, since the probabilities in $\nu$ do not depend on the covariates in $\ell(\nu, \pi; y)$, also the $m$–step for $\nu$ has closed form solution.

2. Obtain a prediction $\hat{s}_i$ for thelatent class membership $s_i$ of each unit $i = 1, \ldots, n$, by assigning $i$ to the class with the highest $Pr(s_i = r | \hat{s}, \hat{y}, y_i) \propto \hat{\nu}_r \prod_{j=1}^{K} \hat{\pi}_{jr}(y_j)^{(s_i y)_j}$, $r = 1, \ldots, R$.

3. Estimate the parameters comprising $\beta$ from a multinomial logistic regression with $\hat{s}_1, \ldots, \hat{s}_n$ as response data.

This three–step procedure provides a simple estimation strategy, which is motivated by its interpretability. However, as discussed in [6] and [25], the resulting estimators for the coefficients in $\beta$ are subject to systematic bias. Motivated by these issues, [6] and [25], recently developed two bias–correction methods relying on a modification of the multinomial log-likelihood for $\hat{s}_1, \ldots, \hat{s}_n$, which incorporates the classification error. The bias–corrected log-likelihood proposed in [6] allows simple estimation via standard algorithms for multinomial logistic regression, but their method can be applied only when the covariates are categorical. A more general correction procedure is considered by [25] to include continuous covariates, improve efficiency, and facilitate wider applicability. There is also a focus on other mechanisms to predict the classes, but the results are not substantially different to those obtained in step 2 [25, 2].

Although the bias adjustment proposed by [25] is widely considered in routine applications, the estimates obtained under three–step routines remain still sub-optimal compared to one–step methods, since they do not directly maximize the full–model log-likelihood (2). Indeed, when the overarching focus is on providing reliable inference for the parameters $\beta$ and $\pi$ in (1), it is arguably more coherent to attempt a direct maximization of the log-likelihood in (2), since it guarantees unbiased, efficient, and consistent estimators of $\beta$ and $\pi$—if the model is correctly specified [6].

2. Nested EM for one–step estimation

To address the issues discussed in Sect. 1.1–1.2, we propose a nested EM algorithm for one–step estimation which avoids approximations of the expected log-likelihood $Q_1(\beta \mid \theta^{(t)})$ for the regression coefficients $\beta_1, \ldots, \beta_{R-1}$, but instead improves this function sequentially via a set of conditional expectation–maximizations for every vector of coefficients $\beta_r, r = 1, \ldots, R - 1$, given the others $\beta_l, l \neq r$. 


Working with the conditional expected log-likelihoods is appealing in providing a set of different logistic regressions for which the Pólya-gamma data augmentation scheme [23] guarantees closed-form maximization based on generalized least squares. Indeed, following Theorem 1 in [23], the generic logistic likelihood \( \exp(\mathbf{x}^\top \mathbf{\beta})^\omega [1 + \exp(\mathbf{x}^\top \mathbf{\beta})]^{-b} \), can be rewritten as \( 2^{-b} \exp[(a - 0.5b)\mathbf{x}^\top \mathbf{\beta}] \cosh(0.5\mathbf{x}^\top \mathbf{\beta}) - b \), \( b \geq 0 \), whereas the likelihood of a Pólya-gamma variable \( \omega \sim \rho(a, \mathbf{x}^\top \mathbf{\beta}) \) is proportional to \( \exp[-0.5 a (\mathbf{x}^\top \mathbf{\beta})^2] \cosh(0.5 \mathbf{x}^\top \mathbf{\beta})^b \). Hence, combining these two quantities provides an augmented likelihood \( \exp[-0.5 a (\mathbf{x}^\top \mathbf{\beta})^2 + (a - 0.5b)\mathbf{x}^\top \mathbf{\beta}] \) for data \((a, \omega)\) which is proportional to the one induced by a Gaussian regression for the transformed response \( \omega^{-1}(a - 0.5b) \sim N(\mathbf{x}^\top \mathbf{\beta}, \omega^{-1}) \), thus allowing simple maximization within a Gaussian framework. We shall notice that other Gaussian-related data augmentations for logistic regression have been developed in the past years [e.g. 12, 16]. However, as discussed in [23], these strategies require either approximations or more complex representations relying on multiple layers of latent variables, thus leading to intractable computations. Instead, the Pólya-gamma data augmentation leads directly to a Gaussian likelihood with a single latent variable \( \omega \), whose expectation is analytically available via \( \mathbb{E}(\omega) = 0.5 b (\mathbf{x}^\top \mathbf{\beta})^{-1} \tanh(0.5 \mathbf{x}^\top \mathbf{\beta}) \).

Beside providing tractable computations, the proposed procedure guarantees the monotonicity for the log-likelihood sequence \( \ell(t^\theta; \mathbf{y}, \mathbf{x}) \), at every \( t \), and is directly motivated by an exact \( \text{EM} \) algorithm for the special case of \( R = 2 \) latent classes, which is described in the next section.

2.1. Exact \( \text{EM} \) algorithm for \( R = 2 \)

Recalling the above discussion, let us first focus on deriving a simple and exact \( \text{EM} \) algorithm for the special case of \( R = 2 \) latent classes, which provides analytical maximization steps also for the coefficients in \( \mathbf{\beta} \). This is obtained by considering an additional set of augmented data leveraging results from the Pólya-gamma data augmentation [23] discussed above. In fact, when \( R = 2 \) the expected value of \( \ell_1(\mathbf{\beta}; s, \mathbf{x}) = \ell_1(\mathbf{\beta}_1; s, \mathbf{x}) \) can be easily rewritten as

\[
Q_1(\mathbf{\beta} | \theta^0) = Q_1(\mathbf{\beta}_1 | \theta^0) = \sum_{i=1}^n \log \left[ \frac{\exp(\mathbf{x}^\top \mathbf{\beta}_1) \omega_i}{[1 + \exp(\mathbf{x}^\top \mathbf{\beta}_1)]} \cdot \frac{[1 + \exp(\mathbf{x}^\top \mathbf{\beta}_1)]}{1 + \exp(\mathbf{x}^\top \mathbf{\beta}_1)} \right] = \sum_{i=1}^n \log \left[ \frac{\exp(\mathbf{x}^\top \mathbf{\beta}_1) \omega_i}{1 + \exp(\mathbf{x}^\top \mathbf{\beta}_1)} \right],
\]

to obtain the log-likelihood \( \ell_1^*(\mathbf{\beta}_1; s^0(\mathbf{x}), \mathbf{x}) \) of a particular logistic regression in which the entries in \( s^0(\mathbf{x}) \) act as response data, and those in \( \mathbf{x} \) as predictors. This result allows the implementation of the Pólya-gamma data augmentation for logistic regression summarized in Sect. 2. In particular, defining \( b := 1, a := \tilde{s}^0_i(\mathbf{x}), \mathbf{x}^\top \mathbf{\beta} := \tilde{s}_i^0 \mathbf{\beta}_1 \) and \( \omega := \omega_{i1} \), provides the complete log-likelihood

\[
\ell_1^*(\mathbf{\beta}_1; s^0(\mathbf{x}), \mathbf{x}, \omega) = \sum_{i=1}^n \left[ \frac{\cosh(0.5(\mathbf{x}_i^\top \mathbf{\beta}_1))}{\exp(0.5 \omega_{i1}(\mathbf{x}_i^\top \mathbf{\beta}_1) - 2)} \cdot \frac{\exp[(\tilde{s}_i^0 - 0.5)\mathbf{x}_i^\top \mathbf{\beta}_1]}{\cosh(0.5(\mathbf{x}_i^\top \mathbf{\beta}_1))} \right] + \text{const},
\]

\[
= \sum_{i=1}^n \left[ -0.5 \omega_{i1}(\mathbf{x}_i^\top \mathbf{\beta}_1)^2 + (\tilde{s}_i^0 - 0.5)\mathbf{x}_i^\top \mathbf{\beta}_1 \right] + \text{const},
\]

(7)

for \( s^0(\mathbf{x}), \mathbf{x} \), and the Pólya-gamma augmented data \( \omega = (\omega_{i1}, \ldots, \omega_{in}) \). Equation (7) is a simple quadratic function of \( \mathbf{x}_i^\top \mathbf{\beta}_1 \), and is linear in the augmented Pólya-gamma data. This allows the implementation of a simple nested expectation step, in which every augmented data \( \omega_{i1} \) is replaced with the expectation \( \mathbb{E}(\omega_{i1} | s^0(\mathbf{x})_i, \mathbf{y}, \mathbf{x}_i) := \bar{\omega}_{i1} = 0.5(\mathbf{x}_i^\top \mathbf{\beta}_1)^{-1} \tanh(0.5 \mathbf{x}_i^\top \mathbf{\beta}) \) of the Pólya-gamma variable \( \rho(a, 1, \mathbf{x}_i^\top \mathbf{\beta}_1) \), for each \( i = 1, \ldots, n \), to obtain \( Q_1(\mathbf{\beta}_1 | \theta^0) = \)
\[ \sum_{i=1}^{n} -0.5 \tilde{\omega}_i^{(t)} (\tilde{\eta}_i^{(t)} - x_i^T \beta_1)^2 + \text{const}, \quad \text{with } \tilde{\eta}_i^{(t)} = (\tilde{s}_i^{(t)} - 0.5) / \tilde{\omega}_i^{(t)}. \] The appealing property associated with this nested expected log-likelihood \( Q_1(\beta_1 \mid \theta^{(t)}) \), compared to \( Q(\beta_1 \mid \theta^{(t)}) \), is that it allows direct maximization for the coefficients in \( \beta_1 \). Indeed, exploiting the generalized least squares, \( Q(\beta_1 \mid \theta^{(t)}) \) is analytically maximized at

\[ \beta_1^{(t+1)} = (X^T \tilde{\Omega}^{(t)} X)^{-1} X^T \tilde{\Omega}^{(t)} \tilde{\eta}^{(t)}, \]  

where \( X \) is the \( n \times P \) matrix having rows \( x_i^T \), whereas \( \tilde{\Omega}^{(t)} = \text{diag}(\tilde{\omega}_1^{(t)}, \ldots, \tilde{\omega}_n^{(t)}) \) and \( \tilde{\eta}^{(t)} = (\tilde{\eta}_1^{(t)}, \ldots, \tilde{\eta}_n^{(t)})^T \). To highlight the benefits of equation (8), let us relate it to the corresponding updating step of the Newton–Raphson in [11, 24]—i.e. \( \beta_1^{(t+1)} = \beta_1^{(t)} + (X^T \Lambda^{(t)} X)^{-1} X^T (s_i^{(t)} - \tilde{y}_i^{(t)}(x)) \)—and the monotone EM algorithm in [4]—i.e. \( \beta_1^{(t+1)} = \beta_1^{(t)} + [X^T \text{diag}(0.25, \ldots, 0.25) X]^{-1} X^T (s_i^{(t)} - \tilde{y}_i^{(t)}(x)) \). In particular, adding and subtracting \( X \beta_1^{(t)} \) inside \( \tilde{\eta}^{(t)} \), we obtain

\[ \beta_1^{(t+1)} = (X^T \tilde{\Omega}^{(t)} X)^{-1} X^T \tilde{\Omega}^{(t)} (\tilde{\eta}^{(t)} + X \beta_1^{(t)} - X \beta_1^{(t)}) = \beta_1^{(t)} + (X^T \tilde{\Omega}^{(t)} X)^{-1} X^T \tilde{\Omega}^{(t)} (s_i^{(t)} - 0.5 \mathbf{1} - \tilde{\Omega}^{(t)} X \beta_1^{(t)}), \]

(9)

after noticing that each element in \( s_i^{(t)} - 0.5 \mathbf{1} - \tilde{\Omega}^{(t)} X \beta_1^{(t)} \) can be easily rewritten as \( z_i^{(t)} - 0.5 - \omega_i^{(t)} x_i^T \beta_1^{(t)} = z_i^{(t)} - 0.5 [1 + \tanh(0.5 x_i^T \beta_1^{(t)})] - 0.5 [1 + \exp(-s_i^{(t)})][1 + \exp(s_i^{(t)})]^{-1} = z_i^{(t)} - (1 + \exp(-s_i^{(t)}))^{-1} = z_i^{(t)} - \tilde{y}_i^{(t)}(x) \).

Hence, in contrast to the uniform lower bound \(-X^T \text{diag}(0.25, \ldots, 0.25) X\) derived by [4], equation (9) relies on an adaptive one \(-X^T \tilde{\Omega}^{(t)} X\), which is formally induced by a Pólya-gamma data augmentation and, therefore, is expected to improve computational efficiency, without affecting monotonicity. Indeed, these properties are confirmed by our empirical studies in Sect. 3, and by the theoretical results in Proposition 2.1. Also the Newton–Raphson algorithm in [11, 24] effectively allows \(-X^T \Lambda^{(t)} X\) to change at each iteration. However, the routine has no monotone convergence.

We shall also stress that, although we obtained \( Q_1(\beta_1 \mid \theta^{(t)}) \) sequentially, this quantity can be directly interpreted as the expectation of the complete log-likelihood \( \ell_1(\beta_1; \mathbf{s}, \mathbf{x}, \omega) \). Hence, since \( Q_2(\mathbf{x} \mid \theta^{(t)}) \) is analytically maximized in (6), and does not depend on the Pólya-gamma data, the resulting routine is an exact EM algorithm based on the complete log-likelihood \( \ell_1(\beta_1; \mathbf{s}, \mathbf{x}, \omega) = \ell_1(\beta_1; \mathbf{s}, \mathbf{x}, \omega) + \ell_2(\mathbf{x}, \mathbf{y}, \mathbf{s}) \). Finally, note that since \( \pi^{(t+1)} \) can be easily obtained before updating the \( \beta \) coefficients, a more efficient computational procedure, inspired by the multi-cycle expectation conditional maximization algorithm [22], is to update also the expectation of the augmented data \( s_1, \ldots, s_n \) based on \( \pi^{(t+1)} \) instead of \( \pi^{(t)} \), before applying (8). This solution will be adopted in the general case \( R > 2 \), discussed below.

### 2.2. Nested EM algorithm for \( R > 2 \)

When more than two latent classes are considered, \( Q_1(\beta \mid \theta^{(t)}) \) has a multinomial logit structure, and not a logistic one. Therefore, a direct application of the Pólya-gamma data augmentation is not possible. However, as we will outline, the conditional expected log-likelihood for every vector of coefficients \( \beta_r, \; r = 1, \ldots, R-1 \), given the others \( \beta_1 \), \( l \neq r \), can be rewritten as a proper logistic log-likelihood [e.g. 16], thus motivating a Pólya-gamma data augmentation.

Consistent with this consideration, we propose a nested EM routine, improving the expected log-likelihood for \( \beta \), via a set of conditional expectation–maximizations for each vector \( \beta_r, \; r = 1, \ldots, R-1 \), given the others \( \beta_1 \), \( l \neq r \). In particular, for each iteration \( t \), we consider \( R' = R - 1 \) nested cycles which sequentially improve the conditional expected log-likelihood of one vector of coefficients, keeping fixed the others at their most recent value. Therefore, let
where the constants \( a \), \( \beta \), and \( \theta \) denote the estimates for the class-specific vectors of coefficients at cycle \( r = 1, \ldots, R \) in iteration \( t \), we seek a sequential updating procedure providing the chain inequalities

\[
Q_l(\beta^{(r+1)/R}) | \beta^{(r+1)/R}, \beta^{(r-1)/R}) \geq Q_l(\beta^{(r+1)/R}) | \beta^{(r+1)/R}, \beta^{(r-1)/R}), \quad \text{for each } r = 1, \ldots, R. \tag{10}
\]

In equation (10) the key difference between \( \beta^{(r+1)/R} \) and \( \beta^{(r+1)/R} \), is that only the class-specific vector of coefficients \( \beta \), is updated, whereas all the others are kept fixed. Hence, at every cycle \( r \) we seek to improve the expected log-likelihood produced in \( r - 1 \), by modifying only the value of \( \beta \), from its previous estimate at \( t \) to a new one at \( t + 1 \). In this respect, such strategy partially recalls the idea underlying the univariate version of the Newton–Raphson in [26], and adapts it to blocks of parameters in order to obtain more efficient updates relying on the most recent estimates.

Moreover, as outlined in Proposition 2.1, the sequential improvements underlying the nested \( \text{em} \), along with the direct maximization of \( Q_2(\pi | \theta^{(t)}) \), additionally guarantee monotonicity in the log-likelihood sequence \( \ell(\beta^{(t)}, \pi^{(t)}, y, x) \). This is a key property to ensure reliable convergence [4]. Note that in equation (10), also the expectation of the conditional log-likelihood, with respect to the augmented data, is sequentially updated using the estimates of the coefficients from the previous cycle, in the same spirit of the multi-cycle expectation conditional maximization algorithm [22].

In deriving the updating procedure for the regression coefficients in \( \beta \), which has property (10), we adapt the results outlined for the case \( R = 2 \), providing simple and explicit maximization procedures for each \( \beta \).

Focusing on the cycle \( r \), within iteration \( t \), let \( Q_l(\beta_r | \theta^{(r+1)/R}) \), with \( \theta^{(r+1)/R} = (\pi^{(t+1)}, \beta^{(r+1)/R}) \) denote the conditional expected log-likelihood, written as a function of only \( \beta_r \), with all the other class-specific coefficients fixed at their corresponding estimates at cycle \( r - 1 \). According to equations (4) and (5), the function \( Q_l(\beta_r | \theta^{(r+1)/R}) \) equals to

\[
\sum_{i=1}^{n} \left\{ \sum_{l \neq r} \exp(x_i^T \beta_r) \log \left[ \frac{\exp(x_i^T \beta_r)}{\exp(x_i^T \beta_r) + c_i^{(r+1)/R}} \right] + \sum_{l \neq r} \exp(x_i^T \beta_r) \log \left[ \frac{\exp(x_i^T \beta_r)}{\exp(x_i^T \beta_r) + c_i^{(r+1)/R}} \right] \right\}, \tag{11}
\]

where the constants \( c_i^{(r+1)/R} \) denote the sum of all the exponential quantities \( \exp(x_i^T \beta_r) \), \( l \neq r \), written as a function of the current estimates for the class-specific coefficients vectors at cycle \( r - 1 \), whereas the expectation of the augmented latent class indicators are calculated in (5) as a function of \( \pi^{(t+1)} \) and \( \beta^{(r+1)/R} \).

Since we aim to improve \( Q_l(\beta_r | \theta^{(r+1)/R}) = Q_l(\beta^{(r+1)/R}) | \theta^{(r+1)/R}) \) by updating the current estimate of \( \beta_r \), under the Pólya-gamma data augmentation outlined in the previous section, let us highlight a logistic log-likelihood in (11). In particular, holding out additive constants not depending on \( \beta_r \), and dividing both the numerator and the denominator of the arguments in the logarithmic functions by the quantities in the vector \( c^{(r+1)/R} \), we easily obtain:

\[
Q_l(\beta_r | \theta^{(r+1)/R}) = \sum_{i=1}^{n} \log \left\{ \frac{\exp(x_i^T \beta_r - a_i^{(r+1)/R})}{1 + \exp(x_i^T \beta_r - a_i^{(r+1)/R})} \right\} + \text{const}, \quad \text{with } a_i^{(r+1)/R} = \log c_i^{(r+1)/R}, \tag{12}
\]

given that \( x_i^{(r+1)/R} + \sum_{l \neq r} y_i^{(r+1)/R} = 1 \). Hence, up to the constants \( a_i^{(r+1)/R} \) in the linear predictor, equation (12) for \( \beta_r \), has the same form of the expected log-likelihood for \( \beta_1 \) discussed in Sect. 2.1, thereby motivating the Pólya-gamma data augmentation at each cycle \( r \) of the nested \( \text{em} \) routine. In particular, introducing \( \omega_r \sim \text{PG} \{ 1, x_i^T \beta_r - a_i^{(r+1)/R} \} \), for every statistical unit \( i = 1, \ldots, n \), we can easily rely on the same analytical results in Sect. 2.1, to show
that the conditional expectation of each $\omega_r$ is
\[
\bar{\omega}_{ir}^{(r+1)/R'} = 0.5(\bar{X}^T \bar{\eta}_{ir}^{(r+1)/R'} - a_i^{(r+1)/R'})^{-1} \tanh[0.5(\bar{X}^T \bar{\eta}_{ir}^{(r+1)/R'} - a_i^{(r+1)/R'})],
\]
and that the desired increment (10) at cycle $r$, can be simply obtained—similarly to (8)—by setting
\[
\beta_r^{(r+1)} = (X^T \Omega^{(r+1)/R} X)^{-1} X^T \bar{\Omega} \bar{\eta}_{ir}^{(r+1)/R'},
\]
where $\Omega^{(r+1)/R} = \text{diag}(\omega_{ir}^{(r+1)/R}), \ldots, \omega_{ir}^{(r+1)/R})$, whereas $\bar{\eta}_{ir}^{(r+1)/R'} = (\bar{\eta}_{ir}^{(r+1)/R}, \ldots, \bar{\eta}_{ir}^{(r+1)/R})^T$, with
\[
\bar{\eta}_{ir}^{(r+1)/R'} = (\bar{\omega}_{ir}^{(r+1)/R'} - 0.5 + \omega_{ir}^{(r+1)/R'}, \omega_{ir}^{(r+1)/R'}(\bar{\omega}_{ir}^{(r+1)/R'} - 1))\Omega^{(r+1)/R}\bar{\eta}_{ir}^{(r+1)/R'}.
\]

Algorithm 1 provides the detailed guideline for the implementation of our computational routine to maximize the log-likelihood $\ell(\beta, \pi, y, x)$ in equation (2). Note that all the expectations and maximizations steps rely on simple and exact expressions, in contrast with current computational methods for latent class models with covariates. Moreover, as discussed in Proposition 2.1, our methods guarantee monotonicity in the log-likelihood sequence.

**Proposition 2.1.** The nested EM routines developed in Sect. 2.2 imply $\ell(\beta^{(r+1)}, \pi^{(r+1)}, y, x) \geq \ell(\beta^{(r)}, \pi^{(r)}, y, x)$ for any $t$.

**Proof.** To prove Proposition 2.1, we first need to ensure that our nested conditional expectation–maximizations for the regression coefficients $\beta_r, r = 1, \ldots, R'$, meet property (10). Since each of these optimizations steps is a pure EM algorithm based on the Polya-gamma data augmentation, following [10], we have
\[
\ell_r(\beta_r^{(r+1)}, \pi_r^{(r+1)/R'}, x) \geq \ell_r(\beta_r^{(r)}, \pi_r^{(r+1)/R'}, x), \quad \text{for each } r = 1, \ldots, R',
\]
implying $Q_1(\beta^{(r+1)/R'} \mid \beta^{(r+1)/R'}) \geq Q_1(\beta^{(r+1)/R'} \mid \beta^{(r+1)/R'})$, provided that in (12) these two log-likelihoods differ by an additive constant which does not depend on $\beta$. Therefore, to conclude the proof, we need to ensure that the chain inequalities in (10), along with the direct maximization of $Q_2(\pi \mid \theta^{(r)})$, guarantee the inequality $\ell(\beta^{(r+1)/R'}, \pi^{(r+1)}, y, x) \geq \ell(\beta^{(r)}, \pi^{(r)}, y, x)$. Let $Q(\beta, \pi \mid \theta^{(r)}) = Q_2(\pi \mid \theta^{(r)}) + Q_2(\pi \mid \theta^{(r)})$ denote the expected log-likelihood, written as a function of all the parameters in our statistical model. Direct maximization of $Q_2(\pi \mid \theta^{(r)})$ in the first step of our routine, guarantees $Q_1(\pi^{(r+1)} \mid \beta^{(r+1)}, \pi^{(r)}) \geq Q_1(\pi^{(r+1)}, \pi^{(r)} \mid \beta^{(r+1)}, \pi^{(r)})$. Therefore, as discussed in page 165 of [21], this first result guarantees $\ell(\pi^{(r+1)}, \beta^{(r+1)}, y, x) \geq \ell(\pi^{(r+1)}, \beta^{(r+1)}, y, x)$. Similarly, the inequalities in (10), characterizing each nested cycle $r$, ensure $\ell(\pi^{(r+1)}, \beta^{(r+1)/R'}, y, x) \geq \ell(\pi^{(r+1)}, \beta^{(r+1)/R'}, y, x)$ for every $r = 1, \ldots, R'$. Joining these results we can prove...
Proposition 2.1 via the inequalities:

\[
\ell(\pi^{(t)}, \beta_1^{(t)}, \ldots, \beta_r^{(t)}; y, x) \leq \ell(\pi^{(t+1)}, \beta_1^{(t+1)}, \ldots, \beta_r^{(t+1)}; y, x) \leq \ldots \leq \ell(\pi^{(t+1)}, \beta_1^{(t+1)}, \ldots, \beta_r^{(t+1)}; y, x) \leq \ldots \leq \ell(\pi^{(t+1)}, \beta_1^{(t+1)}, \ldots, \beta_r^{(t+1)}; y, x).
\]

2.3. Hybrid nested EM for one–step estimation

Before evaluating empirical performance of the nested EM and comparing results with relevant competitors, we first propose a more practical and efficient version of our routine. Indeed, as discussed in [25], the EM is characterized by stable maximization even when the initialization is far from the optimal solution, whereas Newton–Raphson methods guarantee fast convergence when the routine is close to the maximum. Motivated by this result, we propose a simple modification of the nested EM to improve computational efficiency, without substantially affecting maximization.

In particular, the proposed hybrid procedure starts with the nested EM presented in Sect. 2.2, and performs maximization as in Algorithm 1, until the log-likelihood sequence is close to reach a global—or local—maximum. Then, when the increment \(\ell(\beta^{(i+1)}, \pi^{(i+1)}; y, x) - \ell(\beta^{(i)}, \pi^{(i)}; y, x)\) is less or equal to a pre-selected small \(\epsilon\), the \(m\)-step for the coefficients in \(\beta\) switches to the Newton–Raphson updating procedure discussed in Sect. 1.1. Although the inclusion of the Newton–Raphson methodology could still cause possible decays in the log-likelihood sequence, when the routine is in a small neighborhood of the global—or local—maximum, the parabolic approximation is more stable.

3. Empirical study

To evaluate the benefits associated with the proposed nested EM in a real–data application, we compare the computational performance of our EM with the results obtained under the popular routines outlined in Sect. 1.1 and 1.2.

In particular, one–step competitors comprise the EM algorithm with one Newton–Raphson step (nrEM) from [3], the more formal EM routine (nrEMQ1) maximizing \(Q_l(\beta \mid \theta^{(i)})\) as in [11, 24], and the conservative version of the nrEMQ1 which relies on the rescaled updating of \(\beta\), as outlined in Sect. 1.1, with \(\alpha = 0.5\) (nrEMQ1, \(\alpha = 0.5\)). Based on the discussion in Sect. 1.1, we additionally adapted the lower–bound mm algorithm (mmEM) proposed by [4, 5] to compare empirical performance with a routine guaranteeing monotone log-likelihood sequences. The three–step methods considered are instead the classical strategy (3stepClassical) discussed in Sect. 1.2 [e.g. 8], and the bias–corrected algorithm (3stepCorrection) from [25]. We do not implement the routine in [6], since the covariates enter as continuous variables in the application considered. Moreover [25] is more widely used, and does not provide substantially different estimates compared to [6], according to the simulations in [25]. The HybridEM is instead the modification of our NestedEM presented in Sect. 2.3. In performing maximization under this modified version of the nested EM we set \(\epsilon = 0.01\). Although we have found the results robust to moderate changes in small values of \(\epsilon\), it is important to notice that high \(\epsilon\) values should be avoided since they allow the hybrid algorithm to rely on Newton–Raphson methods even when \(\ell(\beta^{(i)}, \pi^{(i)}; y, x)\) is far from the maximum.

To provide a detailed computational assessment, we perform estimation under the above algorithms for 100 runs, with varying random initialization. The routines are all initialized at the same starting values—for each run—and stop...
Table 1. Election data with \( R = 2 \) latent classes: Performance assessments comparing the maximization quality and the computational efficiency of the algorithms discussed in Sect. 1.1, 1.2 and Sect. 2.

| \( R = 2 \) ELECTION DATA | \( \text{NR}_{\text{EM}} \) | \( \text{NR}_{\text{EM}}Q_1 \) | \( \text{NR}_{\text{EM}}Q_1 \), \( \alpha = 0.5 \) | \( \text{MM}_{\text{EM}} \) |
|--------------------------|----------------|----------------|----------------|--------------|
| Number of runs with a decay in \( \ell(\theta); y, x \) | 48 | 18 | 4 | 0 |
| Number of runs reaching a local mode | 60 | 19 | 3 | 0 |
| \(|\ell(\theta); y, x) - \max_x(\ell(\theta); y, x)\)| local modes | 645.786 | 778.587 | 778.587 | NA |
| Iterations to reach \( \max_x(\ell(\theta); y, x) \) | 104 | 106 | 122 | 139 |
| Averaged computational time for each run | 0.048” | 0.076” | 0.099” | 0.098” |

| \( R = 2 \) ELECTION DATA | \( 3\text{STEP}_\text{Classical} \) | \( 3\text{STEP}_\text{Correction} \) | \( \text{NESTED}_{\text{EM}} \) | \( \text{HYBRID}_{\text{EM}} \) |
|--------------------------|----------------|----------------|--------------|--------------|
| Number of runs with a decay in \( \ell(\theta); y, x \) | NA | NA | 0 | 0 |
| Number of runs reaching a local mode | 100 | 100 | 0 | 0 |
| \(|\ell(\theta); y, x) - \max_x(\ell(\theta); y, x)\)| local modes | 17.672 | 12.199 | NA | NA |
| Iterations to reach \( \max_x(\ell(\theta); y, x) \) | NA | NA | 109 | 106 |
| Averaged computational time for each run | 0.074” | 0.063” | 0.107” | 0.095” |

when the increment in the log-likelihood is lower than \( 10^{-11} \). For every run we study the maximization performance, and the computational efficiency of the different algorithms. Specifically, the maximization performance is monitored by the number of runs with a decay in the log-likelihood sequence, and by the frequency of runs converging to local modes. For the runs reaching local modes, we also compute the median of the difference between the log-likelihood in these local modes and the maximum one. Computational efficiency is instead studied via the median number of iterations for convergence, computed only for the runs reaching \( \max_x(\ell(\beta, \pi; y, x)) \), and the averaged computational time.\(^1\) Code to reproduce the analyses in Sect. 3.1 is available at https://github.com/danieledurante/nEM.

3.1. Performance in a real–world application to election data

Tables 1 and 2 summarize the maximization performance and the computational efficiency of the algorithms discussed in Sect. 1.1, 1.2 and Sect. 2, for an application to the election data available in the R library polCA [19]. This tutorial dataset measures voters political affiliation, along with their opinions on how well six different personality traits describe the presidential candidates Al Gore and George Bush before the 2000 US presidential elections. These \( J = 12 \) categorical opinions are collected on a four items scale for \( n = 880 \) voters. Following the analyses in [19] we assess the performance of the different maximization algorithms considering both \( R = 2 \) and \( R = 3 \) latent classes, with the political affiliation variable entering as covariate in the multinomial logistic regression for such latent classes.

Consistent with the left panel in Fig. 1, and the results in Proposition 2.1, the proposed \( \text{NESTED}_{\text{EM}} \) and the \( \text{MM}_{\text{EM}} \) for one–step estimation always provide a monotone sequence for the full–model log-likelihood (2) in Table 1, thereby guaranteeing an accurate maximization and a reduced frequency of local modes. Including one Newton–Raphson step, as in the algorithms proposed by [3] and [11, 24], leads instead to decays in the log-likelihood sequences, which increase the chance to reach local modes far from \( \max_x(\ell(\beta, \pi; y, x)) \). As discussed in Sect. 1.1, this issue is more severe for the \( \text{SR}_{\text{EM}} \) procedure proposed by [3] compared to the more formal \( \text{SR}_{\text{EM}}Q_1 \) approach in [11, 24]. The reduced maximization performance associated with these Newton–type algorithms is mitigated by a partial improvement in the computational efficiency compared to the monotone \( \text{NESTED}_{\text{EM}} \) and the \( \text{MM}_{\text{EM}} \), which remain, however,

\(^1\)Computations rely on a simple R (version 3.3.2) implementation in a machine with one Intel Core i5 2.5 GHz processor and 4 GB of RAM.
two separate maximizations, not directly related to \( \ell \) increasing the number of classes leads to a more complex log-likelihood surface, which requires finer maximization log-likelihoods which are substantially below the true one. A reason for this poor maximization performance, is that causing convergence to local modes in several runs. It is also worth noticing how these local modes are associated with one–step algorithms relying on Newton–Raphson experience again frequent decays in the log-likelihood sequence, making it impossible to study the number of iterations to reach max \((\hat{\beta}, \pi)\) \(\ell(\beta, \pi, y, x))\). Therefore, since these algorithms perform estimation in fractions of seconds, an improvement in the maximization performance is arguably the most important property. Note also that combining the \(\text{nestedEM}\) with the \(\text{naEMQ}_1\), provides an \(\text{hybridEM}\) which guarantees the accurate maximization performance characterizing the monotone algorithms and a computational efficiency comparable to the Newton–type methods.

Rescaling the Newton–Raphson updating of \(\beta\) by \(\alpha = 0.5\), allows improvements in the maximization performance, but these gains are associated with a reduced computational efficiency. Indeed, more reliable convergence routines are obtained for \(\alpha = 0.5\), however these improvements are not sufficient to obtain the same performance of the \(\text{nestedEM}\), and the \(\text{hybridEM}\), while providing a lower computational efficiency compared to our routines. To conclude the evaluation of the one–step algorithms, we shall notice that the lower–bound correction proposed by [4, 5] effectively guarantees monotone log-likelihood sequences and reliable convergence, but their global conservative bound requires more iterations to reach convergence compared to the \(\text{nestedEM}\) and the \(\text{hybridEM}\).

As discussed in Sect. 1.2, the three–step estimation algorithms do not attempt direct maximization of the full–model log-likelihood (2). The consequences of this choice are evident in Table 1 with all the runs of the \(3\text{stepClassical}\) and the \(3\text{stepCorrection}\) routines providing sub-optimal estimates which produce log-likelihoods of the full model always below the maximum one. Therefore, these methods converge systematically to local modes, making it impossible to study the number of iterations to reach \(\max_{\beta,\pi}\ell(\beta, \pi, y, x))\).

Therefore, these methods converge systematically to local modes, making it impossible to study the number of iterations to reach \(\max_{\beta,\pi}\ell(\beta, \pi, y, x))\). Also the number of decays in the sequence \(\ell(\beta^{(t)}, \pi^{(t)}; y, x)\) is somewhat irrelevant to evaluate the three–step methods, since the estimation routines are based on two separate maximizations, not directly related to \(\ell(\beta^{(t)}, \pi^{(t)}; y, x)\). This has also an effect on the computational time.

According to Table 2, increasing the number of latent classes to \(R = 3\) provides similar conclusions. In particular, one–step algorithms relying on Newton–Raphson experience again frequent decays in the log-likelihood sequence, causing convergence to local modes in several runs. It is also worth noticing how these local modes are associated with log-likelihoods which are substantially below the true one. A reason for this poor maximization performance, is that increasing the number of classes leads to a more complex log-likelihood surface, which requires finer maximization

| ELECTION DATA R = 3 | 3stepClassical | 3stepCorrection | nestedEM | hybridEM |
|----------------------|---------------|----------------|----------|----------|
| Number of runs with a decay in \(\ell(\theta^{(t)}; y, x)\) | NA | NA | 0 | 0 |
| Number of runs reaching a local mode | 100 | 100 | 24 | 25 |
| \(|\ell(\hat{\theta}; y, x)\)–max_{\theta}\ell(\theta; y, x)| | 42.224 | 39.104 | 0.644 | 0.644 |
| Iterations to reach \(\max_{\theta}\ell(\theta; y, x))\) | NA | NA | 171 | 166 |
| Averaged computational time for each run | 0.229” | 0.212” | 0.359” | 0.265” |

| ELECTION DATA R = 3 | \(\text{naEMQ}_1\) | \(\text{naEMQ}_1\) \(\alpha = 0.5\) | \(\text{mmEM}\) |
|----------------------|----------------|----------------|----------|
| Number of runs with a decay in \(\ell(\theta^{(t)}; y, x)\) | 78 | 37 | 12 | 0 |
| Number of runs reaching a local mode | 94 | 51 | 24 | 27 |
| \(|\ell(\hat{\theta}; y, x)\)–max_{\theta}\ell(\theta; y, x)| | 830.046 | 1105.626 | 4.894 | 0.644 |
| Iterations to reach \(\max_{\theta}\ell(\theta; y, x))\) | 146 | 151 | 161 | 229 |
| Averaged computational time for each run | 0.073” | 0.182” | 0.230” | 0.283” |
algorithms for reliable estimation. This is also evident when comparing the maximization performance of the three-step methods in the Table 1 and Table 2. Also the three monotone algorithms experience local modes, but their total number is comparable to the conservative \( \alpha \text{EMQ}_1 \) with \( \alpha = 0.5 \), and the associated log-likelihoods are much closer to the maximum. Consistent with Table 1, the computational efficiency of the different algorithms remains in general on a comparable scale both for the number of iterations to convergence, and for the averaged computational time.

In performing the above assessments we initialized the \( \beta \) from independent Gaussians with mean 0 and small variance 0.5. We shall notice that, reducing such variance—i.e. initializing \( \beta \) very close to 0—yield to improvements in the above routines, including the Newton–type ones. A possible reason for this result is that such initialization provides equal class probabilities as initial values, thus starting the routines from a more central region in the parametric space. Also in these cases, however, the performance of the \text{neSTmEM} and the \text{hybrIDmEM} was not worse than the other routines, while being less sensitive to initialization. Similar conclusions were obtained in other real data applications.

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