Iterative proportional scaling revisited:  
a modern optimization perspective

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Abstract

This paper revisits the classic iterative proportional scaling (IPS) from a modern optimization perspective. In contrast to the criticisms made in the literature, we show that based on a coordinate descent characterization, IPS can be slightly modified to deliver coefficient estimates, and from a majorization-minimization standpoint, IPS can be extended to handle log-affine models with features not necessarily binary-valued or nonnegative. Furthermore, some state-of-the-art optimization techniques such as block-wise computation, randomization and momentum-based acceleration can be employed to provide more scalable IPS algorithms, as well as some regularized variants of IPS for concurrent feature selection.

1 Introduction

1.1 Background

Count data are ubiquitous in modern statistical applications. Such data are often cross-classified into contingency tables, where iterative proportional scaling (IPS) can be applied as a standard tool (Fienberg and Meyer, 2006). IPS was firstly introduced by Deming and Stephan (1940) to adjust a contingency table to obey prescribed column and row marginals, the problem of which is referred to as matrix raking nowadays. In general, IPS can be applied to Kullback–Leibler (KL) divergence minimization with linear constraints, and Poisson log-linear model fitting on multi-way tables (Ireland and Kullback, 1968; Bishop et al., 1975), and there is an interesting
duality between these two types of problems (Good, 1963; Csiszár, 1975). Theoretical studies regarding the convergence properties of IPS undergo a long history and we refer to Pukelsheim (2014) for a comprehensive survey. To name a few, Fienberg (1970) took a geometric approach, assuming that all entries in the input table are positive, while Haberman (1974) and Bishop et al. (1975) were among the first to use the ascent property of the associated log-likelihood. It is worth mentioning that the theoretical studies become more challenging if IPS operates on a table with zero entries (Sinkhorn and Knopp, 1967; Csiszár, 1975).

Although the standard version of IPS is derived for contingency tables, it has some quite useful and popular extensions. For example, Darroch and Ratcliff (1972) proposed the generalized iterative scaling (GIS) which can fit Poisson log-affine models with non-negative designs. Later, Pietra et al. (1997) developed a more relaxed improved iterative scaling (IIS), without the requirement that all rows of the design matrix must sum to one. The class of IPS algorithms are widely used in the areas of Markov random fields and Gibbs distributions, natural language processing, matrix factorization, econometrics, boosting, and others (Sinkhorn, 1964; McCallum et al., 2000; Lahr and De Mesnard, 2004; Phillips et al., 2004; Kurras, 2015).

Today, IPS is less frequently used by statisticians, largely due to the outstanding performance and generality of Newton-type algorithms. In fact, Newton-Raphson is the default routine in most software for fitting generalized linear models (GLMs), and can have quadratic convergence in contrast to the linear convergence rate of IPS (ignoring the cost difference per iteration). Consider a five-way table of size $10 \times 10 \times 10 \times 10 \times 10$. The associated Poisson model including all up to three-way interactions has 8,146 independent parameters. The corresponding Hessian matrix has more than $10^7$ entries, leading to prohibitively high computational cost when using Newton-Raphson. Quasi-Newton methods are more computationally economical, but still fail easily when the model is of high dimensionality. First-order methods (such as gradient descent) are typically more scalable; in our problem, however, there exists no universal stepsize due to the unbounded Hessian. This means that some line search method must be adopted, but frequent function and gradient evaluations can be expensive on big data.

The traditional IPS algorithm is potentially helpful in this regard. In comparison with Newton-type and gradient descent methods, IPS has certain benefits in computation. We illustrate the procedure via a toy example. Consider a three-way table $m_{ijk}$ of size $m_1 \times m_2 \times m_3$ with the
categorical variables denoted by $X, Y, Z$ and assume a Poisson log-linear model ($XY, YZ, XZ$) with margins $m_{ij+}, m_{i+k}$ and $m_{+jk}$ as sufficient statistics (Agresti, 2012). Starting with initial counts $[\mu_{ijk}^{(0)}]_{1 \leq i \leq m_1, 1 \leq j \leq m_2, 1 \leq k \leq m_3}$, IPS adjusts the estimated counts in a multiplicative manner iteratively:

$$
\mu_{ijk}^{(t+1/3)} = \mu_{ijk}^{(t)} m_{ij+}/\mu_{ij+}^{(t)} \quad \text{for all } (i, j), \quad \mu_{ijk}^{(t+2/3)} = \mu_{ijk}^{(t+1/3)} m_{i+k}/\mu_{i+k}^{(t+1/3)} \quad \text{for all } (i, k), \quad \mu_{ijk}^{(t+1)} = \mu_{ijk}^{(t+2/3)} m_{+jk}/\mu_{+jk}^{(t+2/3)} \quad \text{for all } (j, k) \text{ in the } t\text{-th epoch.}
$$

Clearly, all calculations are “in-place” (with no need of auxiliary variables) and no line search is required. The procedure has memory efficiency, scalability and implementation ease. In addition, it converges within one step once the solution has a closed form expression.

IPS is subject to some serious criticisms in the literature. Although IPS produces expected cell counts, it does not deliver any coefficient estimate nor asymptotic covariance estimate. The elegant scaling procedure has however a somewhat narrow scope and may encounter difficulties say in the scenarios with features not necessarily bi-leveled or nonnegative, or in shrinkage estimation. Finally, though cost-effective per iteration, IPS often requires a large number of iterations to converge.

This paper attempts to investigate IPS from a modern optimization perspective to improve and generalize the classic method and overcome the aforementioned obstacles. Our main contributions are threefold. First, we are able to show that IPS implicitly involves a coefficient-update step and adding it back leads to a novel coordinate descent characterization of the procedure. To the best of our knowledge, this is the first fix of IPS to produce coefficient estimates. Second, we reveal an interesting connection of IPS to majorization-minimization (MM) algorithms (Hunter and Lange, 2004). The MM principle successfully generalizes IPS to handle arbitrary features, with the celebrated GIS and IIS taken as two particular instances. Third, we employ some state-of-the-art optimization techniques, such as block-wise computation, randomization and momentum-based acceleration, to develop highly scalable IPS algorithms (without using parallel computation), as well as some sparse variants of IPS for concurrent feature selection.

The rest of the paper is organized as follows. Notations and model assumptions are introduced in Section 1.2. Section 2 describes a coefficient-driven IPS based on coordinate descent, and discusses its convergence properties, efficient implementation and acceleration. Section 3 shows several effective ways of constructing MM surrogate functions to generalize IPS. Section 4 develops sparse IPS for high dimensional estimation. Section 5
shows the accuracy and efficiency brought by blockwise descent, randomization, reparametrization, and momentum-based acceleration in simulations and real data experiments.

After the acceptance of our paper, we noticed the work by Anna and Tamás (2015), which showed how to update the coefficients in IPS under the assumption of strictly positive counts. In Section 2 we give a more general result and more efficient algorithms. They also proposed two generalized procedures for multinomial likelihood optimization based on bisection or coarse-to-fine search. See Section 3 for some fast optimization algorithms that can operate on general designs.

1.2 Notation and model setting
Notation. Given \( N \in \mathbb{N} \), we define \([N] = \{1, 2, \ldots, N\}\). We use bold lower-case and upper-case symbols to denote column vectors and matrices, respectively, i.e. \( \mathbf{x} = [x_i] \in \mathbb{R}^N \) and \( \mathbf{X} = [x_{ij}] \in \mathbb{R}^{N \times p} \), where \( i \in [N] \) and \( j \in [p] \). The inner product between two vectors \( \mathbf{x} \) and \( \mathbf{y} \) is \( \langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y} \), their Hadamard product is denoted by \( \mathbf{x} \odot \mathbf{y} \), and their component-wise division is denoted by \( \mathbf{x} \oslash \mathbf{y} \). Given any matrix \( \mathbf{X} \), we denote by \( x_{i+} \) the \( i \)th row sum \( \sum_j x_{ij} \). For notational ease, we extend all scalar functions and operations in a component-wise manner. For example, given \( \mathbf{x} = [x_i] \in \mathbb{R}^N \) and \( \mathbf{y} \in \mathbb{R}^N \), \( \exp(\mathbf{x}) \) stands for \([\exp(x_i)]\), \( \log(\mathbf{x}) = [\log x_i] \), and \( \mathbf{x} \succeq \mathbf{y} \) indicates that \( x_i \geq y_i \) for all \( i \in [N] \). The design matrix \( \mathbf{X} \in \mathbb{R}^{N \times p} \) is frequently partitioned into columns (features) and rows: \( \mathbf{X} = [\mathbf{x}_1 \ldots \mathbf{x}_p] = [\mathbf{x}_1^T \ldots \mathbf{x}_N^T]^T \) with \( \mathbf{x}_j \in \mathbb{R}^N \) and \( \mathbf{x}_i \in \mathbb{R}^p \). Given two square matrices \( \mathbf{X} \) and \( \mathbf{Y} \), \( \mathbf{X} \succeq \mathbf{Y} \) means \( \mathbf{X} - \mathbf{Y} \) is positive semi-definite. We denote by \( \|\mathbf{x}\|_1 \) and \( \|\mathbf{x}\|_2 \) the \( \ell_1 \)-norm and the \( \ell_2 \)-norm of \( \mathbf{x} \), respectively. The spectral norm and the infinity norm of a matrix \( \mathbf{X} \) are defined as \( \|\mathbf{X}\|_2 = \sigma_{\text{max}}(\mathbf{X}) \) (the largest singular value of \( \mathbf{X} \)) and \( \|\mathbf{X}\|_\infty = \max_i \sum_j |x_{ij}| \), respectively. Given \( \mathbf{a}, \mathbf{b} \in \mathbb{R}^N \) with \( a_i, b_i \geq 0 \), the (generalized) KL divergence is defined by \( D_{\text{KL}}(\mathbf{a}||\mathbf{b}) = \sum_{i=1}^N (a_i \log(a_i/b_i) - a_i + b_i) \) and takes \(+\infty\) when \( a_i \neq 0 \) and \( b_i = 0 \) for some \( i \). The conventions \( \log 0 = -\infty \), \( 0 \log(0/0) = 0 \), and \( 0 \cdot (\pm \infty) = 0 \) are adopted.

Given a contingency table model, one can vectorize all cell counts and introduce a design matrix in the framework of Poisson log-affine models. Concretely, let \( X_k \) \((1 \leq k \leq r)\) be the \( k \)th categorical variable taking values in \([m_k] \) and \( r \) be the total number of categorical variables. Introduce dummy variables \( X_k^{(\ell_k)} \triangleq I(X_k = \ell_k) \) for \( \ell_k = 2, 3, \ldots, m_k \) with \( X_k = \ell_1 \) as
the baseline, and let \( X_k = [X_k^{(2)}, X_k^{(3)}, \ldots, X_k^{(m_k)}] \). Then the model matrix containing all main effects has form \([1, X_1, X_2, \ldots, X_r]\). Similarly, the model matrix including all two-way interactions has the following form \([X_1 \times X_2, \ldots, X_1 \times X_r, X_2 \times X_3, \ldots, X_2 \times X_r, \ldots, X_{r-1} \times X_r]\), where \( X_j \times X_k \triangleq [X_j^{(2)} X_k^{(2)}, \ldots, X_j^{(m_j)} X_k^{(m_k)}], \ldots, X_j^{(m_j)} X_k^{(m_k)}] \). Higher-order interactions can be included as well. Given an arbitrary \( X \) where \( \bar{\gamma} \) tor. In some applications, e.g., rate data analysis and matrix ranking, an extra offset \( q \) mean \( \mu \) the criterion strongly convex, cf. Section 2.2.1. Given an arbitrary \( X \in \mathbb{R}^{N \times p} \), a log-linear model with mean \( \mu \in \mathbb{R}^N \) satisfies \( \mu = \exp(X \beta) \), where \( \beta \) denotes the coefficient vector. In some applications, e.g., rate data analysis and matrix ranking, an extra offset \( q \geq 0 \) is required to specify a log-affine model (Lauritzen, 1996): \( \mu = q \circ \exp(X \beta) \) or \( \mu_i = q_i \exp(\tilde{x}_i^T \beta) \). We allow \( \beta_j \) to take \( \pm \infty \), i.e., \( \beta \in \mathbb{R}^p \) with \( \mathbb{R} = [-\infty, \infty] \) (the extended real line). Throughout the paper, we will not consider overdispersion or inflated zeros.

Let \( n \in \mathbb{R}^N \) with \( n_i \geq 0 \) denote the observed entries. The maximum likelihood (ML) estimation problem of \( \mu \) according to the log-affine model can be formulated by

\[
\min_{\mu} l(\mu) \triangleq -\langle n, \log \mu \rangle + \langle 1, \mu \rangle \quad \text{s.t.} \quad \mu = q \circ \exp(\eta), \eta \in \overline{R}_X,
\]

where \( \overline{R}_X = \{\sum_{j=1}^p \beta_j x_j : \beta \in \mathbb{R}\} \) denotes the closure of the range of \( X \). Equivalently, the loss can be \( D_{KL}(n||\mu) \) or the deviance function. For convenience, the constraint region is denoted by \( \mathcal{M} \triangleq \{\mu \mid \mu = q \circ \exp(\eta), \eta \in \overline{R}_X\} \). As suggested by Lauritzen (1996), theoretically it is more convenient to consider (1) in a slightly more restricted manner in order to guarantee the convergence of IPS:

\[
\min_{\mu} D_{KL}(n||\mu) \quad \text{s.t.} \quad \mu \in \mathcal{M} \cap \mathcal{M}^*,
\]

where \( \mathcal{M}^* \triangleq \{\mu \mid l(\mu) < +\infty\} \), meaning that \( n_i > 0 \) implies \( \mu_i > 0 \) (\( 1 \leq i \leq N \)).

For simplicity, the following assumptions are made throughout the paper:

(i) \( n \neq 0 \), (ii) \( x_j \neq 0 \), \( \forall j \in [p] \), (iii) \( \tilde{x}_i \neq 0 \), \( \forall i \in [N] \), (iv) \( \bar{\mathcal{M}} \cap \mathcal{M}^* \neq \emptyset \).

Assumption (i) is trivial. (ii) and (iii) are without loss of generality, since one can drop the corresponding trivial predictors and/or observations. (iv) ensures finite likelihood for at least one point in \( \bar{\mathcal{M}} \), and typically holds in real-life applications (otherwise one could add a mild \( \ell_2 \)-type penalty to make the criterion strongly convex, cf. Section 2.2). It is worth mentioning that, under (iv), one can remove certain observations to ensure a positive \( q \) without affecting the coefficient estimation. In fact, for any \( \mu = [\mu_i] \in \mathcal{M} \cap \mathcal{M}^* \),
\( q_i = 0 \) implies \( \mu_i = 0 \) and \( n_i = 0 \); so the \( i \)th observation does not contribute to the objective function in (1) and can be excluded in optimization. This can greatly simplify computation and analysis.

To extend IPS, we specify three types of design matrices:

\[(a) \, x_{ij} = 0 \text{ or } 1 \text{ (binary)}, \quad (b) \, x_{ij} \geq 0 \text{ (non-negative)}, \quad (c) \, x_{ij} \in \mathbb{R} \text{ (general)}.\] (3)

Clearly, design matrices derived from contingency table models are special cases of (a). But real applications can go much beyond this binary setting.

## 2 A Coordinate Descent Characterization

As mentioned in Section 1, IPS is commonly used for matrix raking to find a table \( \mu \) that not only matches the marginals of a reference table \( n \in \mathbb{R}^N \) but is closest to an initial (prior) \( q \in \mathbb{R}^N \) in the sense of relative entropy or KL divergence:

\[
\min_{\mu \in \mathbb{R}^N} D_{KL}(\mu || q) = \sum_{i=1}^{N} \left[ \mu_i \log(\mu_i/q_i) - \mu_i + q_i \right], \quad \text{s.t. } \langle x_j, \mu \rangle = \langle x_j, n \rangle, \quad j \in [p].
\]

(4)

The features \( x_j \) are binary-valued in the table setup (but not so in general) and \( \langle x_j, n \rangle \) give prescribed marginals. In certain applications there is no need to provide \( n \), since only the constraint values are needed. When \( 1 \in \mathcal{R}(X) \), \( \langle 1, \mu \rangle \) is a constant and so the objective can be reduced to \( \sum \mu_i \log(\mu_i/q_i) \).

Without the binary restriction on the design, (4) defines the general problem of maximum entropy with linear constraints, and has widespread applications in statistical mechanics, information theory, natural language processing, and ecology (Berger et al., 1996; Dudík et al., 2004; Elith et al., 2011). The duality between the maximum entropy problem (4) and the maximum likelihood problem (1) is well known by statisticians, and indeed many take the ML route to study the properties of IPS.

### 2.1 Coefficient-driven IPS

IPS is often criticized for not being able to deliver a coefficient estimate. We will show, however, that this is not true and IPS includes an implicit coefficient-update step.
First, although the objective function of IPS is conventionally formulated with respect to the unknown mean vector \( \mu \) (or \( \log \mu \)) in the literature, it is arguably more insightful to rewrite (1) in terms of \( \beta \):

\[
\min_{\beta \in \mathbb{R}^p} l(\beta) = -\langle n, X \beta \rangle + \langle q, \exp(X \beta) \rangle,
\]

where we used \( \mu_i(\beta) = q_i \exp(\tilde{x}_i^T \beta) \). The convenience can be partially observed from the initialization condition of IPS (Fienberg and Meyer, 2006), which requires \( \mu^{(0)} \) to take the form of \( q \circ \exp(\eta^{(0)}) \) for some \( \eta^{(0)} \) in \( \mathcal{R}_X \). Here, we still use \( l(\cdot) \) to denote the loss by abuse of notation, and when \( 1 \in \mathcal{R}(X) \), it is easy to see that (5) amounts to minimizing the \( G^2 \)-statistic

\[
2 \sum n_i \log(n_i/\mu_i(\beta)).
\]

For this convex optimization problem, we can design a simple cyclic coordinate descent (CD) algorithm, which updates \( \beta_j \) (\( 1 \leq j \leq p \)) according to the following formula with the other coordinates fixed

\[
\beta_j^{(t+1)} = \arg \min_{\beta_j} l(\beta_1^{(t+1)}, \ldots, \beta_j^{(t+1)}, \beta_{j+1}, \ldots, \beta_p^{(t)}).
\]

(6)

Define \( \mu^{(t,j-1)} \triangleq q \circ \exp(X \beta^{(t,j-1)}) \) with \( \beta^{(t,j-1)} \triangleq [\beta_1^{(t+1)}, \ldots, \beta_{j-1}^{(t+1)}, \beta_j^{(t)}, \beta_{j+1}, \ldots, \beta_p^{(t)}]^T, j \in [p] \). It is easy to show that \( \beta_j^{(t+1)} \) satisfies the equation

\[
(\mu^{(t,j-1)})^T \{x_j \circ \exp[x_j(\beta_j - \beta_j^{(t)})]\} - x_j^T n = 0.
\]

(7)

Algorithm 1 shows the details of the cyclic coordinate update. The solution to (7) has a closed form in some cases. For example, if we assume the design is derived from a contingency table model, or more generally, \( X \) is binary (cf. (3)), then the following crucial fact

\[
x_{ij} \exp(x_{ij} \beta_j) = x_{ij} \exp(\beta_j)
\]

implies that \( x_j \circ \exp[(\beta_j - \beta_j^{(t)})x_j] = x_j \exp(\beta_j - \beta_j^{(t)}) \), and so

\[
\beta_j^{(t+1)} = \beta_j^{(t)} + \log[x_j^T n/(x_j^T \mu^{(t,j-1)})].
\]

(9)

Step 5 in Algorithm 1 then becomes

\[
\mu^{(t,j)} = \mu^{(t,j-1)} \circ \exp\{x_j \log[(x_j^T n)/(x_j^T \mu^{(t,j-1)})]\},
\]

(10)

or equivalently, \( \mu_i^{(t,j)} = ((x_j, n)/(x_j, \mu^{(t,j-1)})) \mu_i^{(t,j-1)} \) if \( x_{ij} = 1 \), and \( \mu_i^{(t,j)} = \mu_i^{(t,j-1)} \) otherwise (\( 1 \leq i \leq N \)), which is exactly the IPS algorithm used
Algorithm 1 IPS-CD

Input $n$, $q$ and $X$

Initialize $\beta^{(0)} \in \mathbb{R}^p$, $t \leftarrow 0$

1: while not converged do
2: $\mu^{(t,0)} \leftarrow q \circ \exp(X \beta^{(t)})$
3: for $j = 1, 2, \cdots, p$ do
4: $\beta^{(t+1)}_j \in \arg \min_{\beta_j} l(\beta_1^{(t+1)}, \ldots, \beta_{j-1}^{(t+1)}, \beta_j, \beta_{j+1}^{(t)}, \ldots, \beta_p^{(t)}).$ Binary case: cf. (9)
5: $\mu^{(t,j)} \leftarrow \mu^{(t,j-1)} \circ \exp[x_j(\beta^{(t+1)}_j - \beta^{(t)}_j)].$ Binary case: cf. (10)
6: end for
7: $\beta^{(t+1)} \leftarrow [\beta_1^{(t+1)}, \ldots, \beta_p^{(t+1)}]^T$, $t \leftarrow t + 1$
8: end while
9: return $\hat{\mu} = \mu^{(t-1,p)}, \hat{\beta} = \beta^{(t)}$

in matrix raking. In the literature, Haberman (1974) shows that IPS is a cyclic ascent method in updating $\log \mu$, but to the best of our knowledge, formulating IPS as cyclic CD on $\beta$ is new.

Algorithm 1 provides more flexibility in initialization. For instance, $\mu^{(0)} = q$ is unnecessary; rather, starting with an arbitrary $\beta^{(0)} \in \mathbb{R}^p$ suffices. In our experience, a properly chosen initial point can reduce the computational time substantially in large-scale data problems. The algorithm not only offers an easy fix of IPS to yield $\hat{\beta}$, but also suggests efficient ways to update multiple components of $\mu$ at one time. Concretely, when $\beta_j$ ($1 \leq j \leq p$) is changed, all the $\mu_i$ with $x_{ij} \neq 0$ can be updated. It is thus extremely helpful in implementation to consolidate the features and use a design matrix with full column rank (which can be easily obtained by QR or LU decomposition). For example, on the aforementioned homogeneous association model $(XY, XZ, YZ)$ with $X, Y, Z$ taking two levels, each epoch of the ordinary IPS updates all cell values according to the minimal sufficient statistics in $4 \times 3 = 12$ steps (cf. Section 1.1), while IPS-CD updates $\beta$ and the associated cells in 7 steps; see Figure 1 for an illustration.

Some people conjectured that IPS attempted to minimize Pearson’s $X^2$-statistic, but this is not true—see Theorem 1. It is well known that $X^2$ converges faster than $G^2$ to the asymptotic $\chi^2$-distribution. Nicely, our coordinate descent standpoint can modify IPS in a simple way to solve the problem $\min_{\mu} \sum_i [n_i - \mu_i(\beta)]^2 / \mu_i(\beta)$ with $\mu_i(\beta) = q_i \exp(\tilde{x}_i^T \beta)$. In fact, similar to the derivation of (7), given the other coordinates $\beta_j^{(t+1)}$ can be updated...
for a resultant iterative scaling of and with a binary design, the equation has a closed-form solution and the values in 12 steps to satisfy prescribed margins, while (b) updates by solving the equation

\[
\beta \left( I_m \right) \text{ margins as minimal sufficient statistics. Here, } \beta_0 \text{ is the intercept and } \beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6 \text{ denote the coefficients of } I(X = 2), I(Y = 2), I(Z = 2), I(X = 2, Y = 2), I(X = 2, Z = 2) \text{, and } I(Y = 2, Z = 2), \text{ respectively. In each epoch, (a) updates the cell values in 12 steps to satisfy prescribed margins, while (b) updates } \beta \text{ and the associated } \mu_{i,j,k} \text{ in 7 steps.}
\]

by solving the equation

\[
\sum_i x_{ij} \mu_i^{(t,j-1)} \exp[x_{ij} (\beta_j - \beta_j^{(t)})] - \sum_i x_{ij} n_i^2 / \{ \mu_i^{(t,j-1)} \exp[x_{ij} (\beta_j - \beta_j^{(t)})] \} = 0,
\]

and with a binary design, the equation has a closed-form solution and the resultant iterative scaling of } \mu \text{ is

\[
\mu^{(t,j)} = \mu^{(t,j-1)} \circ \exp\left\{ \frac{1}{2} x_j \log [x_j^T (n \circ n) \circ \mu^{(t,j-1)}] / (x_j^T \mu^{(t,j-1)}) \right\}.
\]

The procedure can be conveniently used for testing associations and interactions in contingency tables. Its differences from the ordinary version (10) are seen in the term } n \circ n \circ \mu^{(t,j-1)} \text{ in place of } n, \text{ and the additional factor of } 1/2.

\section{2.2 Convergence properties}

The CD characterization facilitates theoretical studies of the convergence properties of IPS. First, we have a natural outcome for Algorithm 1 for a general design } X .

Theorem 1. For the sequence of iterates } \{ \beta^{(t)} \}_{t=0}^{\infty} \text{ generated by Algorithm 1, the associated function values } l(\beta^{(t)}) \text{ are monotonically non-increasing for } t \geq 0. \text{ In particular, if the first column of } X \text{ corresponds to the intercept,
then the $G^2$-statistic evaluated on $\mu^{(t,1)}$, i.e., $2 \sum_n n_i \log(n_i/\mu^{(t,1)}_i)$, is monotonically non-increasing.

Similar results have been obtained on contingency tables (e.g., Bishop et al. (1975)). The theorem directly follows from the coordinate descent nature of the algorithm design, and is not restricted to tables. Moreover, because of the convexity of the problem, under some regularity conditions, the convergence of the sequence of iterates is readily at hand.

**Theorem 2.** Suppose that there exists a unique solution $\hat{\beta}$ to problem (5) of finite norm. Then the sequence of iterates $\{\beta^{(t)}\}_{t=0}^{\infty}$ generated by Algorithm 1 has a unique limit point $\hat{\beta}$, and the rate of convergence is at least linear.

The linear convergence rate was shown by Fienberg (1970) for matrix ranking. Our theorem builds upon the theory of descent methods (Luo and Tseng, 1992). In consideration of recent advances (Tseng, 2001; Razaviyayn et al., 2013), one can possibly relax the assumption of Theorem 2 in certain ways, but we will not pursue further in this work. We refer to Fienberg and Rinaldo (2012) and Wang et al. (2016) for detailed studies of the existence and uniqueness of MLE. In practice, we could add a mild ridge-type penalty (cf. Section 4), which ensures the condition and enhances numerical stability.

### 2.3 Randomization and block-wise computation

Recently, CD algorithms have received a lot of attention in statistics (high dimensional statistics, in particular) due to their simplicity and low-complexity operations at each iteration. But the characteristic of not updating all variables together may also make them take more iterations and require more stringent conditions to converge. Instead of the cyclic update in Algorithm 1, one can choose the coordinate with the largest derivative in magnitude, $j = \arg \max_j |\nabla_j l(\beta^{(t)})|$, the so-called Gauss-Southwell (G-S) rule. G-S can successfully reduce the number of iterations, and has been analyzed in depth in the literature (see, e.g., Bertsekas (2015) and Nutini et al. (2015)). However, it is inefficient in large problems since all partial derivatives have to be computed—indeed, with the full gradient vector available, one could update the whole vector $\beta$ at each step.

An effective way to speed the convergence of the algorithm is to randomize it. The recent analysis of Nesterov (2012) shows that random coordinate selection can achieve the same convergence rate as G-S. It is worth mentioning
Algorithm 2 A-IPS.

Input $n$, $q$ and $X$

Initialize $\beta^{(0)} \in \mathbb{R}^p$, $t \leftarrow 0$

1: while not converged do
2: $\mu^{(t,0)} \leftarrow q \circ \exp(X \beta^{(t)})$
3: for $j$ in $\text{Perm}[p]$ do
4: $\beta^{(t+1)}_j \in \text{arg min}_\beta l(\beta^{(t+1)}_1, \ldots, \beta^{(t+1)}_{j-1}, \beta_j, \beta^{(t)}_{j+1}, \ldots, \beta^{(t)}_p)$
5: $\mu^{(t,j)} \leftarrow \mu^{(t,j-1)} \circ \exp[x_j(\beta^{(t+1)}_j - \beta^{(t)}_j)]$
6: end for
7: $\beta^{(t+1)} \leftarrow [\beta^{(t+1)}_1, \ldots, \beta^{(t+1)}_p]^T$, $t \leftarrow t + 1$
8: end while
9: return $\hat{\mu} = \mu^{(t-1,p)}$, $\hat{\beta} = \beta^{(t)}$

that random strategies make complexity bounds much easier to obtain, and are often suitable for modern computational architectures. Experience shows that random sampling without replacement (Wright, 2015) works well in IPS. Concretely, at the start of each cycle, we randomly shuffle the elements in $[p]$ to obtain a new index set $\text{Perm}[p]$, and then update the permuted coordinates sequentially. The randomized algorithm, denoted by Accelerated-IPS (A-IPS), is presented in Algorithm 2. In theory, randomized coordinate selection is able to avoid worst-case order of coordinates, and seems to be better than the cyclic rule in an average sense (Richtárik and Takáč, 2014). (Sampling the coordinates in a data-dependent manner may be better, but it involves more computation and is not considered here.)

Extending the coordinate-by-coordinate update to block-by-block update may save some computational time, too. Block coordinate descent (BCD) decomposes all unknowns into $m$ blocks, and updates only one block at a time. In this way, a large difficult problem can be reduced to a series of smaller and easier sub-problems so that Newton or quasi-Newton methods such as L-BFGS (Liu and Nocedal, 1989) can be applied with ease. In the block setting, again, G-S takes much fewer iteration steps than the plain cyclic rule, but in terms of total computational time, it incurs significantly more overhead in big data applications due to the calculation of the full gradient. Perhaps surprisingly, we found that some well-known random rules, such as (block) resampling without replacement, may not have satisfactory performance, either. We recommend random blocking followed by cyclic update, and this random block-wise IPS is referred to as B-IPS. See Figure 2 for an illustration. At the beginning of each iteration, all coordinates are randomly
shuffled and sequentially assigned into \( m \) blocks with sizes \( g_1, \ldots, g_m \), and then we update the blocks of coefficients in a cyclic manner. This strategy substantially outperforms the other rules according to our experiments.

\section{A Majorization-Minimization Viewpoint}

This section uses the majorization-minimization (MM) principle to study and generalize IPS. We refer to 
Lange et al. (2000) and Hunter and Lange (2004) for more details on MM algorithms. Rather than directly minimizing \( l(\beta) \) in (5), our goal here is to construct a surrogate function \( g(\beta \mid \beta^-) \), with \( \beta^- \) denoting the value of \( \beta \) from the last iteration, such that the following properties are satisfied for all \( \beta \in \mathbb{R}^p \):

\[
g(\beta \mid \beta^-) \geq l(\beta), \quad g(\beta \mid \beta) = l(\beta). \tag{11}\]

Then, if we set \( \beta^{(t+1)} \in \arg\min_\beta g(\beta \mid \beta^{(t)}) \), the sequence of iterates satisfies

\[
l(\beta^{(t+1)}) \leq g(\beta^{(t+1)} \mid \beta^{(t)}) \leq g(\beta^{(t)} \mid \beta^{(t)}) = l(\beta^{(t)}). \]

Hence repeatedly minimizing the surrogate function \( g(\cdot \mid \beta^-) \) guarantees the original objective function \( l(\beta) \) to be monotonically non-increasing. Because the problem under consideration is convex, there are other nice properties of the MM iterates (e.g., Chapter 12 of Lange (2013)). We shall focus on the derivation of surrogate functions in this section. For notational simplicity, define \( \mu^- \triangleq \exp(X\beta^-) \) and \( \mu^{(t)} \triangleq \exp(X\beta^{(t)}) \). After getting \( \beta^{(t+1)} \), one can update \( \mu \) by

\[
\mu^{(t+1)} = \mu^{(t)} \circ \exp[\sum_j x_j(\beta_j^{(t+1)} - \beta_j^{(t)})], \tag{12}\]
which still results in an iterative scaling procedure and could be viewed as a generalized IPS.

3.1 GIS and extensions

We derive three surrogate functions all of which are applicable under the non-negative design setting \((3)\). Recall the objective function:

\[
l(\beta) = \sum_i [q_i \exp(\tilde{x}_i^T \beta) - n_i \tilde{x}_i^T \beta] \triangleq \sum_i l_i. \tag{13}
\]

Noticing the convexity of \( l_i \) in \( \beta \), we can apply Jensen’s inequality

\[
l_i = -n_i \tilde{x}_i^T \beta + q_i \exp\{\sum_j \alpha_{ij} \frac{x_{ij}}{\alpha_{ij}} (\beta_j - \beta^-)\} + \tilde{x}_i^T \beta^-
\]

\[
\leq -n_i \tilde{x}_i^T \beta + \sum_j \alpha_{ij} q_i \exp\{\frac{x_{ij}}{\alpha_{ij}} (\beta_j - \beta^-)\} + \tilde{x}_i^T \beta^-
\]

\[
= -n_i \tilde{x}_i^T \beta + \sum_j \alpha_{ij} \mu_i^- \exp\{\frac{x_{ij}}{\alpha_{ij}} (\beta_j - \beta^-)\}, \tag{14}
\]

where \( \alpha_{ij} \) satisfy \( \alpha_{ij} \geq 0, \sum_{j=1}^p \alpha_{ij} = 1 \) for all \( i \). We will not allow \( \alpha_{ij} \) to be zero when \( x_{ij} \neq 0 \). If \( x_{ij} = 0 \), the associated term \( x_{ij} \beta_j \) is \( \beta_j \)-independent and so we set \( \alpha_{ij} = 0 \) for such \( x_{ij} \) formally. This gives

\[
l_i \leq -n_i \tilde{x}_i^T \beta + \sum_{\{j: x_{ij} \neq 0\}} \alpha_{ij} \mu_i^- \exp\{\frac{x_{ij}}{\alpha_{ij}} (\beta_j - \beta^-)\}. \tag{15}
\]

Let’s first study binary designs. With the somewhat naive choice \( \alpha_{ij} = 1/p \), we immediately obtain a surrogate satisfying \((11)\):

\[
g_1(\beta \mid \beta^-) = -n^T X \beta + \frac{1}{p} \sum_{ij} \mu_i^- \exp[p x_{ij} (\beta_j - \beta^-)]. \tag{16}
\]

Given any binary design with \( x_{ij} = 0 \) or 1, which covers the contingency table setting, the optimal solution of \( \arg \min_{\beta} g_1(\beta \mid \beta^-) \) is given by:

\[
\beta_j = \beta^- + \frac{1}{p} \log[\frac{x_j^T n}{(x_j^T \mu^-)}], \quad j \in [p].
\]

The updates of parameter and mean are obtained as follows

\[
\beta^{(t+1)} = \beta^{(t)} + \frac{1}{p} \log[(X^T n) \odot (X^T \mu^{(t)})] \tag{17}
\]

\[
\mu^{(t+1)} = \mu^{(t)} \circ (\exp\{\frac{1}{p} X \log[(X^T n) \odot (X^T \mu^{(t)})]\}). \tag{18}
\]
The MM algorithm shares similarities with the IPS defined in Algorithm 1, but differs in two ways. IPS updates the components of $\beta$ sequentially (asynchronously), while (17) updates the entire vector synchronously. Correspondingly, the stepsize in MM algorithm is smaller than that used in standard IPS.

Now we consider non-negative features. Recall (3), where we have $x_{i+} \neq 0$ for all $i$ from assumption (iii) in Section 1.2. Setting $\alpha_{ij} = x_{ij}/x_{i+}$ in (15) yields

$$l_i \leq -\sum_j n_i x_{ij} \beta_j + \sum_j \frac{x_{ij}}{x_{i+}} \mu_i^- \exp[x_{i+}(\beta_j - \beta_j^-)],$$

which leads to another surrogate function

$$g_2(\beta \mid \beta^-) = -n^T X \beta + \sum_{i,j} \frac{x_{ij}}{x_{i+}} \mu_i^- \exp[x_{i+}(\beta_j - \beta_j^-)].$$

The optimal $\beta$ satisfies $\sum_i x_{ij} \mu_i^- \exp[x_{i+}(\beta_j - \beta_j^-)] = \sum_i n_i x_{ij}$ but does not enjoy a closed form solution in general.

We majorize the term $\exp[x_{i+}(\beta_j - \beta_j^-)]/x_{i+}$ further. For any $a, b$ with $0 < a \leq b$ and $t \in \mathbb{R}$, $\exp(at)/a - 1/a \leq \exp(bt)/b - 1/b$. Applying the inequality with $a = x_{i+}$ and $b = \max_{i} x_{i+} = \|X\|_{\infty} \triangleq R$ ($R > 0$ from assumption (iii) in Section 1.2) to (19) gives

$$g_2(\beta \mid \beta^-) = -n^T X \beta + \sum_{i,j} x_{ij} \mu_i^- \left\{ \exp\left[R(\beta_j - \beta_j^-)\right] \frac{R}{R} - \frac{1}{R} + \frac{1}{x_{i+}} \right\}.$$

Now, the optimal solution can be explicitly evaluated: $\beta_j = \beta_j^- + (1/R) \log(x_j^T n / x_j^T \mu^-)$, and the iterates are then given by

$$\beta^{(t+1)} = \beta^{(t)} + \frac{1}{R} \log[(X^T n) \odot (X^T \mu^{(t)})]$$

$$\mu^{(t+1)} = \mu^{(t)} \circ (\exp\left(\frac{1}{R} X \log[(X^T n) \odot (X^T \mu^{(t)})]\right)).$$

(20) is computationally more efficient than (17) in binary scenarios. (For example, for a three-way table of size $2 \times 2 \times 100$, the main-effects model has $p = 102$ and $R = 4$ and so the stepsize in (20) is much larger.) When $R = 1$, the update of $\mu$ corresponds to the GIS by Darroch and Ratcliff (1972). (Darroch & Ratcliff pre-transformed the original design matrix such that all elements are non-negative and all row sums are equal to one.)
The MM viewpoint is able to extend GIS, further, to deal with an arbitrary design matrix. Define the row support by \(S_j^r \triangleq \{i \in [N] | x_{ij} \neq 0\}\), and \(R \triangleq \|X\|_\infty > 0\). Then \(g_\beta (\beta | \beta^-) = -n^T X \beta + \sum_{j \in [p]} \mu_i^{\frac{1}{R}} \exp\left[\frac{x_{ij}}{R}\right] R (\beta_j - \beta^-_j)\). It is also worth mentioning that MM is capable of deriving block-wise reparametrization, IIS, and quadratic surrogates. For example, consider \((\beta_0 \exp(X \beta))\). Let \(\tilde{\alpha}_i \in \mathbb{R}\), \(\tilde{\beta}_i \in \mathbb{R}^{p-1}\) denote the slope vector. Introducing \(\alpha = \beta_0 + \log(q, \exp(X \tilde{\beta}))\), or \(\exp(\alpha) = \langle q, \exp(\beta_0 + X \tilde{\beta}) \rangle = \langle 1, \mu \rangle\), the log function, for any \(\zeta > 0\), we have \(\log(\zeta x) \leq \zeta x - 1\) and this bound is tight.

3.2 Reparametrization, IIS, and quadratic surrogates

In this subsection, we assume that \(X\) contains a column corresponding to the intercept, i.e., \(X = [1 \ X] \in \mathbb{R}^{N \times p}\) and \(\beta^T = [\beta_0 \ \tilde{\beta}^T]\), where the intercept \(\beta_0\) is a scalar and and \(\tilde{\beta} \in \mathbb{R}^{p-1}\) denotes the slope vector. Introducing \(\alpha \triangleq \beta_0 + \log(q, \exp(X \tilde{\beta}))\), or \(\exp(\alpha) = \langle q, \exp(\beta_0 + X \tilde{\beta}) \rangle = \langle 1, \mu \rangle\), \(l(\beta)\) in (5) becomes

\[
l(\beta) = -\langle n, \beta_0 1 + X \tilde{\beta} \rangle + \langle q, \exp(\beta_0 1 + X \tilde{\beta}) \rangle = -\langle n, X \tilde{\beta} \rangle - \langle 1, n \rangle \beta_0 + \exp(\alpha) = -\langle n, X \tilde{\beta} \rangle - \langle 1, n \rangle [\alpha - \log(q, \exp(X \tilde{\beta}))] + \exp(\alpha).
\]

The problem with respect to \(\alpha\) can be solved by \(\exp(\alpha) = \langle 1, n \rangle = \langle 1, \mu \rangle\), which means the optimal \(\beta_0\) satisfies \(\beta_0 = \log(1, n) - \log(q, \exp(X \tilde{\beta}))\). Therefore, it suffices to study the \(\tilde{\beta}\)-optimization:

\[
\min_{\beta_0, \tilde{\beta} \in \mathbb{R}^{p-1}} L(\tilde{\beta}) \triangleq -\langle n, X \tilde{\beta} \rangle + \langle 1, n \rangle \log(q, \exp(X \tilde{\beta})).
\] (22)

An MM algorithm can be developed for (22). Due to the concavity of the log function, for any \(\zeta > 0\), we have \(\log(\zeta x) \leq \zeta x - 1\) and this bound is tight.
with choice $\zeta(x) = 1/x$. Then

$$
L(\hat{\beta}) = -\langle n, \hat{X}\hat{\beta} \rangle + \langle 1, n \rangle \log[\zeta(\langle q, \exp(\hat{X}\hat{\beta}) \rangle)] - \langle 1, n \rangle \log \zeta \\
\leq -\langle 1, n \rangle \log \zeta - \langle n, \hat{X}\hat{\beta} \rangle + \langle 1, n \rangle \log[\zeta(\langle q, \exp(\hat{X}\hat{\beta}) \rangle) - 1].
$$

(23)

Assuming the non-negative setting (3) and applying Jensen’s inequality (15) with $\alpha_{ij} = \hat{x}_{ij}/\hat{x}_{i+}$, we get

$$
g_4(\hat{\beta} | \hat{\beta}^-) = -\langle n, \hat{X}\hat{\beta} \rangle - \langle 1, n \rangle (\log \zeta + 1) + \langle 1, n \rangle \sum_{i \in [N], j \in [p-1]} \hat{\mu}_{ij} \exp[\hat{x}_{i+}(\hat{\beta}_j - \hat{\beta}_{i+})],
$$

(24)

where $\hat{\mu} \triangleq q \circ \exp(\hat{X}\hat{\beta})$ with its past value denoted by $\hat{\mu}^- = q \circ \exp(\hat{X}\hat{\beta}^-)$. The only choice to guarantee that $g_4$ is a surrogate is $\zeta = 1/\langle q, \exp(\hat{X}\hat{\beta}) \rangle$.

Now, minimizing (24) gives $\hat{\beta}_j^{(t+1)}$ ($1 \leq j \leq p - 1$):

$$
\frac{\langle 1, n \rangle}{\langle 1, \hat{\mu}^{(t)} \rangle} \sum_i \hat{x}_{ij} \hat{\mu}_i^{(t)} \exp[\hat{x}_{i+}(\hat{\beta}_j^{(t+1)} - \hat{\beta}_j^{(t)})] = \sum_i n_i \hat{x}_{ij},
$$

(25)

and the corresponding proportional scaling on $\hat{\mu}$ is given by

$$
\hat{\mu}^{(t+1)} = \hat{\mu}^{(t)} \circ \exp[\hat{X}(\hat{\beta}^{(t+1)} - \hat{\beta}^{(t)})].
$$

(26)

Interestingly, this algorithm can be converted to the celebrated IIS (Pietra et al., 1997) that runs on the normalized observed and estimated counts, i.e., $\hat{n} \triangleq n/\langle 1, n \rangle$ and $\hat{\mu} \triangleq \mu/(1, \mu)$.

**Theorem 3.** The sequence of $\{\hat{\beta}^{(t)}\}_{t=0}^{\infty}$ generated from the MM algorithm (25) and (26) coincides with the $\{\hat{\beta}^{(t)}\}_{t=0}^{\infty}$ generated by IIS:

$$
\sum_i \hat{n}_i \hat{x}_{ij} = \sum_i \hat{x}_{ij} \hat{\mu}_i^{(t)} \exp[\hat{x}_{i+}(\hat{\beta}_j^{(t+1)} - \hat{\beta}_j^{(t)})], \quad j \in [p-1]
$$

(27)

$$
\hat{\mu}^{(t+1)} = \hat{\mu}^{(t)} \circ \exp[\hat{X}(\hat{\beta}^{(t+1)} - \hat{\beta}^{(t)})]/\langle \hat{\mu}^{(t)} \circ \exp[\hat{X}(\hat{\beta}^{(t+1)} - \hat{\beta}^{(t)})] \rangle.
$$

(28)

In (25) and (26), neither the normalization operation nor the intercept update is needed during the iteration. One can extract the intercept estimate at the end.
The reparametrized form (22) offers more options in surrogate construction. A pleasing fact is that the term $\langle 1, n \rangle \log \langle q, \exp(\hat{X}\hat{\beta}) \rangle$ has uniformly bounded curvature. Let’s consider a quadratic function $Q$,

$$Q(\hat{\beta} \mid \hat{\beta}^-) = L(\hat{\beta}^-) + \langle \hat{\beta} - \hat{\beta}^-, \nabla L(\hat{\beta}^-) \rangle + \frac{1}{2} (\hat{\beta} - \hat{\beta}^-)^T W (\hat{\beta} - \hat{\beta}^-).$$ (29)

By Taylor expansion, $Q$ is a valid surrogate function provided that

$$\langle 1, n \rangle \hat{X}^T \left[ \text{diag}(\hat{\mu}) - \frac{\hat{\mu} \hat{\mu}^T}{\langle 1, \hat{\mu} \rangle^2} \right] \hat{X} \preceq W, \forall \hat{\mu} \succeq 0.$$ (30)

A straightforward choice is $W = (\langle 1, n \rangle \| \hat{X} \|^2_2 / 2) I$. It can be refined to $W = \langle 1, n \rangle \hat{X}^T (I - 11^T / N) \hat{X} / 2$ (Bohning and Lindsay, 1988) noticing the matrix in the brackets of (30) has an eigenvector 1 associated with eigenvalue 0. Based on our experience, the latter is better in most large problems and will be adopted unless otherwise specified. In either case, the optimal solution of $\min_{\hat{\beta}} Q(\hat{\beta} \mid \hat{\beta}^-)$ is $\hat{\beta}^- - W^{-1} [-\hat{X}^T n + (\langle 1, n \rangle / \langle 1, \hat{\mu}^- \rangle) \hat{X}^T \hat{\mu}^-]$.

Because the last term $(\hat{\beta} - \hat{\beta}^-)^T W (\hat{\beta} - \hat{\beta}^-)/2$ in (29) can be identified as a Bregman divergence $D(\hat{\beta} \mid \hat{\beta}^-)$, (29) falls into the computational framework where Nesterov’s second acceleration scheme applies (Nesterov, 1988). At each step, it uses two auxiliary sequences and adds momentum terms in updating the iterates. It can be shown rigorously that this ingenious approach leads to improved rate of convergence; see, e.g., Tseng (2010). The resulting algorithm (Algorithm 3) is referred to as the Quadratic-surrogate IPS (Q-IPS). It is worth mentioning that this momentum-based acceleration does not add much additional cost in each step but offers significant improvement over IIS and GIS (cf. Section 5).

4 Regularized Estimation

Modern statistical applications often involve a large number of variables, where regularization is necessary to achieve estimation accuracy or model parsimony. For example, one can append an $\ell_2$-type penalty to the negative log-likelihood to handle collinearity:

$$\min f_2(\beta) \triangleq -\langle n, X\beta \rangle + \langle q, \exp(X\beta) \rangle + \frac{\lambda}{2} \sum_{j=2}^{p} \beta_j^2,$$ (31)
Algorithm 3 Q-IPS.

Input $n, q, X$

Initialize $\hat{\beta}^{(0)} \in \mathbb{R}^{p-1}$, $\theta_0 \leftarrow 1$, $t \leftarrow 0$

1: $\hat{\mu}^{(0)} \leftarrow q \circ \exp(\hat{X} \hat{\beta}^{(0)})$, $\hat{\eta}^{(0)} \leftarrow \hat{\beta}^{(0)}$

2: while not converged do

3: $\hat{\alpha}^{(t)} \leftarrow (1 - \theta_t)\hat{\beta}^{(t)} + \theta_t \hat{\eta}^{(t)}$

4: $\hat{\eta}^{(t+1)} \leftarrow \arg \min_{\hat{\beta}} (\nabla_{\hat{\beta}} L(\hat{\alpha}^{(t)}), (\hat{\beta} - \hat{\alpha}^{(t)})) + \theta_t D(\hat{\beta} | \hat{\eta}^{(t)})$

5: $\hat{\beta}^{(t+1)} \leftarrow (1 - \theta_t)\hat{\beta}^{(t)} + \theta_t \hat{\eta}^{(t+1)}$

6: $\hat{\mu}^{(t+1)} \leftarrow \hat{\mu}^{(t)} \circ \exp(\hat{X}(\hat{\beta}^{(t+1)} - \hat{\beta}^{(t)}))$

7: $\theta_{t+1} \leftarrow (\sqrt{\theta_t^4 + 4\theta_t^2} - \theta_t^2) / 2$

8: $t \leftarrow t + 1$

9: end while

10: $\beta_0^{(t)} \leftarrow \log(1, n) - \log(q, \exp(\hat{X} \hat{\beta}^{(t)}))$

11: $\boldsymbol{\mu}^{(t)} \leftarrow \exp(\beta_0^{(t)}) \hat{\mu}^{(t)}$

12: return $\hat{\mu} = \boldsymbol{\mu}^{(t)}$, $\hat{\beta} = [\beta_0^{(t)} \hat{\beta}^{(t)T}]^T$

where $\beta_1$ corresponds to the intercept column and $\lambda \geq 0$ is a regularization parameter. $\lambda$ can be tuned by AIC (Akaike, 1974) but even fixing it at a small value (say 1e-5) often shows improved accuracy. We recommend including such a mild $\ell_2$-penalty in practical applications, especially those with zero counts. Many of the previously developed algorithms can be easily modified to adapt to (31) and the details are not discussed.

Another popular way of regularization is to enforce sparsity, which can help practitioners select a small set of relevant features. The coordinate descent characterization of IPS enables us to develop its sparse variants on contingency tables. Assume a binary design $X$ (cf. (3)) and consider the following problem subject to an $\ell_1$- or $\ell_0$-penalty

$$\min_{\beta} f_1(\beta) \quad \text{or} \quad f_0(\beta) \triangleq -\langle n, X \beta \rangle + \langle q, \exp(X \beta) \rangle + \sum_{j=1}^{p} \lambda_j |\beta_j| \quad \text{or} \quad \sum_{j=1}^{p} \lambda_j 1_{\beta_j \neq 0},$$

where typically $\lambda_1 = 0$ and $\lambda_j = \lambda$ for $2 \leq j \leq p$. The following theorem can be used to derive the coordinate-wise update for (32).

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Theorem 4. Let \( n, x, q \in \mathbb{R}^N \), \( \beta \in \mathbb{R} \), \( \lambda \geq 0 \). Then the solution to the optimization problem \( \min_{\beta \in \mathbb{R}} -\langle n, x \rangle \beta + \langle q, \exp(\beta x) \rangle + \lambda |\beta| \) is given by
\[
\hat{\beta} = \log \{|\langle x, n \rangle - \lambda \cdot \text{sgn}(\langle x, n - q \rangle) / \langle x, q \rangle | \geq \lambda \text{ and } \hat{\beta} = 0 \text{ otherwise}.
\]
Also, a global solution to \( \min_{\beta \in \mathbb{R}} -\langle n, x \rangle \beta + \langle q, \exp(\beta x) \rangle + \lambda \beta \neq 0 \) is \( \hat{\beta} = \log \{|\langle x, n \rangle / \langle x, q \rangle | \geq \lambda \text{ and } 0 \text{ otherwise} \).

We use the \( \ell_1 \)-penalized problem as an example to show how to modify Algorithm 1 to get a sparsity-pursuing IPS (a similar algorithm can be developed in the \( \ell_0 \) case). Let \( \mu^{(t,j-1)} = q \circ \exp(X[\beta_1^{(t+1)}, \ldots, \beta_p^{(t+1)}, \beta_j^{(t)}, \ldots, \beta_p^{(t)}]^T) \).

From Theorem 4, for any \( j : 1 \leq j \leq p, \beta_j^{(t+1)} = \arg \min_{\beta_j} f_1(\beta_1^{(t+1)}, \ldots, \beta_j^{(t)}, \ldots, \beta_p^{(t), t+1}) = \beta_j^{(t+1)} = \beta_j^{(t)} + \log(\{x_j, n - \lambda \cdot \text{sgn}(\delta_{t,j}) \} / (x_j, \mu^{(t,j-1)})) \text{ if } |\delta_{t,j}| \geq \lambda_j \text{ and } 0 \text{ otherwise}.
\]

When the intercept is not subject to any penalty, it can be updated by \( \beta_j^{(t+1)} = \beta_j^{(t)} + \log(\{x_1, n \} / (x_1, \mu^{(t,j)})). \) So the iterative scaling on the mean vector is \( \mu^{(t,j)} = \mu^{(t,j-1)} \circ \exp(x_j(\beta_j^{(t+1)} - \beta_j^{(t)})) \), or \( \mu^{(t,j)} = \mu^{(t,j-1)} \circ \exp(x_j \log(\{x_j, n - \lambda \cdot \text{sgn}(x_j, n - \nu^{(t,j-1)}) \}/(x_j, \mu^{(t,j-1)})) \) if \( |\langle x_j, n - \nu^{(t,j-1)} \rangle | \geq \lambda_j \) and \( \nu^{(t,j-1)} \) otherwise, where \( \nu^{(t,j-1)} = q \circ \exp(x_1, \beta_1^{(t+1)} + \cdots + x_{j-1}, \beta_{j-1}^{(t+1)} + x_j, \beta_j^{(t+1)} + \cdots + x_p, \beta_p^{(t)}) \). This modified Algorithm 1 is termed \( \ell_1 \)-IPS.

In contrast to the greedy procedures for maximum entropy with concurrent feature selection in the literature, our optimization-based algorithm is stable in the sense that there is an associated objective function (32) that is guaranteed to be non-increasing, and no quadratic approximation or line search is required.

5 Experiments

This section tests various algorithms on both contingency tables and log-linear models with non-binary features. The observed vector \( n = [n] \) has independent entries satisfying \( n_i \sim \text{Poi}(\mu_i^*) \) (1 \( \leq i \leq N \)), where the mean vector \( \mu^* = \exp(X \beta^*) \) and the first column of the design matrix \( X \) is assumed to be \( 1 \). The details of how to generate the true coefficient vector \( \beta^* \) will vary in different settings. Given each setting, we simulate 20 data sets and report averaged results. The measures to characterize the computational optimization error and statistical estimation error of the \( t \)-th iterate are the relative gradient \( \|g_t\|_\infty / \|g_0\|_\infty \), and the relative estimation error \( \|\beta(t) - \beta^*\|_2^2 / \|\beta^*\|_2^2 \), where \( g_t \) (\( t \geq 0 \)) is the gradient of the original objective function (5) evalu-
ated at $\beta^{(0)}$. The termination criterion is met if $\|g_t\|_\infty / \|g_0\|_\infty \leq \epsilon_{\text{tol}}$ or the running time is greater than $t_{\text{max}}$. By default, $\epsilon_{\text{tol}} = 1e^{-4}$ and $t_{\text{max}} = 600$. Typically, we will plot computational and statistical errors (on the log scale for better visibility) against computational time, rather than the number of iterations, since different algorithms may have very different per-iteration complexity.

The algorithms for comparison include IPS (cf. Alg. 1), A-IPS (cf. Alg. 2), GIS (cf. (20) & (21)), IIS (cf. (27) & (28)), Newton (Schmidt, 2012), Q-IPS (cf. Alg. 3), and B-IPS on the reparametrized problem (22). The initial value $\beta^{(0)}$ is 0 in all experiments. The block sizes in B-IPS are set to be $g_k = 200$ unless otherwise specified. An efficient implementation of Newton’s method with bracketing line-search can be found in Schmidt (2012). The simulations are conducted on a PC with 2.9GHz CPU, 16GB memory, and 64-bit Windows 10. In the following, we first run IPS algorithms on contingency tables to examine the power of acceleration brought by different randomization strategies, then compare IIS, GIS, Newton-type algorithms and our proposed generalized IPS on problems with non-binary features, as well as studying their scalability on large-scale data. At the end, a real marketing campaign dataset is analyzed with the sparsity-pursuing IPS.

### 5.1 Power of randomization

The first experiment compares different random schemes on a $10 \times 10 \times 10 \times 10$ table with all two-way interactions. This homogeneous association model (Agresti, 2012) has 523 predictors, including 36 main effects and 486 two-way associations in addition to the intercept. The coefficient vector is generated in two ways. In the first setting, the intercept is 2, the last 10 components are sampled independently from $0.5\mathcal{N}(1, 1) + 0.5\mathcal{N}(3, 1)$, and the remaining are 0; in the second setting, we set 30 randomly chosen components of $\beta^*_j$ to nonzero, sampled from the previous mixture distribution, and set the rest zero. The results averaged over 20 runs are shown in Figure 3.

According to the figure, A-IPS is much faster than IPS in the first setting, and is comparable to it in the second setting, but in both scenarios, A-IPS delivers far more statistically accurate estimates. (The optimization and estimation errors are shown on the log scale.) Perhaps surprisingly, fixed blocking with random block selection does not show the full power of randomization. Our random-blocking-based B-IPS is clearly the winner both in computational efficiency and in statistical estimation.
Next, we compare A-IPS and B-IPS with Newton’s method on a table of size $10 \times 10 \times 10 \times 10 \times 10$, where a three-way homogeneous association model including all interactions up to third order is assumed (and thus $p = 8,146$). The coefficients are generated such that $\beta_0^* = 5$, the last 2,000 are independently sampled from $\mathcal{N}(1, 1)$ and the rest zero. Seen from Figure 4, Newton’s algorithm could not deliver a useful estimate within the time limit. It was quite memory-demanding in the experiment. In comparison, A-IPS and B-IPS offer good scalability and statistical accuracy.
5.2 Generalized IPS algorithms

This subsection goes beyond the binary feature setting and we use generalized IPS to handle nonnegative features as well as those having both positive and negative values. By default, the prototype design $\hat{X}$ (the submatrix of $X$ excluding the intercept) is generated with each row sampled independently from $\mathcal{N}(0, [\rho^{j-k}])$, where $\rho = 0.8$ and $1 \leq j, k \leq p - 1$. Some shifting and scaling operations will be performed to avoid overflow issues or to make the design non-negative.

The first experiment is to find the winning algorithm among GIS, IIS, and Q-IPS. The celebrated GIS and IIS only run on non-negative features, which can be produced by $\hat{X} \leftarrow \hat{X} - (\min_{i,j} \hat{x}_{ij}) \mathbf{11}^T$. We scale it down further, $\hat{X} \leftarrow \hat{X} / (50 \| \hat{X} \|_{\max})$, for better numerical stability. An artifact is that the obtained matrix has all row sums approximately equal, which appears too ideal in the real-world. So we multiply each row by a random factor $1 + |z_i|$ with $z_i \sim \mathcal{N}(0, 1)$. The true coefficient vector is generated by $\beta_0^* = 1$ and $\beta_j^* \sim 0.5\mathcal{N}(10, 1) + 0.5\mathcal{N}(-10, 1)$ for $1 \leq j \leq p - 1$. The results shown in Figure 5 are for $N = 1,000$ and $p = 100$, where we plot the algorithm progress (in terms of optimization error and estimation error) as the computational time or iteration number increases. (To better differentiate GIS and Q-IPS, we only show part of the plots.) Although IIS needs fewer iterations, GIS is found to be more efficient than IIS. This is due to the cost of solving $p - 1$ nonlinear equations at each iteration of IIS. We also see that Q-IPS
outperforms GIS and IIS.

Figure 5: Performance comparison between GIS, IIS and Q-IPS ($N = 1,000$, $p = 100$). The top two plots show how optimization and estimator errors change over time, and the bottom two are against the iteration number.

Next, we conduct a larger experiment with $p = 2,000, 4,000$ and $N = 20,000$, to compare Q-IPS and B-IPS with Newton. In generating the simulation data, we scale down the prototype design by $\hat{X} \leftarrow \hat{X}/(20\|\hat{X}\|_{\text{max}})$, and set $\beta^*_j \sim i.d. 0.5\mathcal{N}(10, 1) + 0.5\mathcal{N}(-10, 1)$ for $1 \leq j \leq p - 1$ and $\beta^*_0 = 10$. Figure 6a) demonstrates two typical stages of Newton’s method: the damped Newton phase and the quadratically convergent phase (see Boyd and Vandenberghe (2004)). Though converging super fast in the second stage, in 6b), this algorithm took too long to complete the first stage, thereby perhaps less useful.
in big data applications. In contrast, B-IPS and Q-IPS are able to deliver accurate estimates within the time limit, and B-IPS seems to have better scalability than Q-IPS.

![Graph](a) p = 2,000

![Graph](b) p = 4,000

Figure 6: Performances comparison between Q-IPS, B-IPS and Newton on large non-negative designs with $N = 20,000$, $p = 2,000$ (top), 4,000 (bottom).

Finally, we turn to problems with features not restricted to be nonnegative and compare the performance of Newton, B-IPS and L-BFGS. We set $\beta_0^* = 10$ and $\beta_j^* \sim \mathcal{N}(10, 1) + \mathcal{N}(-10, 1)$ for $1 \leq j \leq p - 1$ and scale the prototype design matrix by $\hat{X} \leftarrow \hat{X}/(100\|\hat{X}\|_{\max})$. Fixing $N = 50,000$, we vary $p$ from 1,000 to 12,000. When $p = 10,000$ or 12,000, not all methods converge fast, and we set a time limit $t_{\max} = 600$. The relative gradient (relGrad) and the estimation error (estErr) are scaled by $1 + 7$ and $1 + 4$, respectively.
respectively, when reported in Table 1.

Table 1: Computational & statistical performances of Newton, B-IPS and L-BFGS on general designs of large size.

|            | \(p = 1,000\) | \(p = 4,000\) | \(p = 10,000\) |
|------------|----------------|----------------|-----------------|
| \(\epsilon_{tol} = 1e-6\) | Time | estErr | Time | estErr | Time | estErr |
| Newton     | 35.2 | 0.12 | 528.7 | 0.11 | – | – |
| B-IPS\(^1\) | 16.8 | 3.2 | 116.4 | 23.2 | 5.92 | 109.3 |
| \(p = 4,000\) | \(p = 10,000\) | \(p = 12,000\) |
| \(\epsilon_{tol} = 1e-6\) | \(t_{max} = 600\) | Time | estErr | relGrad | estErr | Time | estErr |
| L-BFGS     | 276.5 | 2.6 | 12250 | 1022 | – | – |
| B-IPS\(^2\) | 94.2 | 2.8 | 5.6 | 44.1 | 12.8 | 462.8 |

From the table, we notice that B-IPS is less precise than Newton in general, but having low computational complexity makes it suitable for large-scale data applications where moderate accuracy usually suffices. Indeed, Newton’s method, when feasible, gives the smallest estimation error, but it easily fails when \(p\) is large (say \(p \geq 6000\)). B-IPS\(^1\) (with Newton as the sub-problem solver and \(g_k = 200\)) has better efficiency and scalability in computation—see the case when \(p = 10,000\), in particular. The same conclusion can be drawn from the comparison between quasi-Newton and B-IPS. In the experiments, L-BFGS ran out of memory when \(p > 10,000\). B-IPS\(^2\), which takes L-BFGS as the sub-problem solver and \(g_k = 2000\), showed the best scalability. In summary, the benefits brought by BCD, reparametrization, and randomization are impressive in large-scale problems. We conducted even larger experiments (with \(p \geq 20,000\)) to study the scalability of B-IPS; the reader may refer to the Appendix for more details.

5.3 \(\ell_1\)-IPS on real data

The dataset is collected from a Portuguese marketing campaign related to bank deposit subscription (Moro et al., 2014). We use 41,188 instances and 10 categorical variables to study whether a client subscribes a term deposit or not. The information of these variables is shown in Table 2. We group the data at each observed combination level of all categorical variables, and use the total number of successful subscriptions as the response variable.
| Variables | Description |
|-----------|-------------|
| job       | type of job (12 levels) |
| marital   | marital status (4 levels) |
| education | education level (8 levels) |
| default   | whether the client has credit in default (3 levels) |
| housing   | whether the client has housing loan (3 levels) |
| loan      | whether the client has personal loan (3 levels) |
| contact   | contact communication type, cellular or telephone (2 levels) |
| month     | the month in which the last contact was made (10 levels) |
| day       | the day of week when the last contact was made (5 levels) |
| poutcome  | outcome of the previous marketing campaign (3 levels) |

Table 2: Categorical variables in the bank campaign data.

We consider a three-way association model, including all main effects, second-order interactions, and third-order interactions. This results in a large model with 5,874 predictors. We ran $\ell_1$-IPS to compute the solution path as shown in Figure 7 and used EBIC (Chen and Chen, 2008) for parameter tuning, where a sparse model with only 16 predictors was obtained. See Table 3 for the selected terms; we also labeled all main effects in Figure 7. (We ran the experiment on a two-way association model, too, and found that all the main terms and two-way interaction terms listed in Table 3 still got selected.)

Figure 7: Left: the $\ell_1$ solution path on the bank marketing data. Right: the solution path including selected variables only.

Some interesting and useful conclusions can be drawn from the variable
First, month plays an important role in the marketing campaign, as supported by some previous studies (e.g., Moro et al. (2014)). In particular, clients are unlikely to subscribe a term deposit if the last contact occurs in November. Moreover, contact communication type being cellular and the outcome of previous marketing campaign being successful are favorable factors for successful subscription.

According to the table, all of the selected two-way interactions involve the variable poutcome = non-exist (no record in the previous campaign), which separates out this special group of clients. Our model also contains two three-way terms, and notably they show no collinearity with the other selected variables, thereby worthy of consideration. The positive coefficients of the two terms, \( (\text{job} = \text{technician}) \ast (\text{education} = \text{professional}) \ast (\text{marital} = \text{married}) \) and \( (\text{poutcome} = \text{non-exist}) \ast (\text{education} = \text{univ}) \ast (\text{marital} = \text{single}) \), indicate that the group of married technicians who received professional training and the group of singles with university-level degrees but no record in the previous marketing campaign tend to subscribe a term deposit.

| Main | month = mar (+) | month = may (−) | month = oct (+) | month = nov (−) | education = univ (+) | poutcome = success (+) | default = unkown (−) | contact = telephone (−) | loan = yes (−) |
|------|-----------------|-----------------|-----------------|-----------------|----------------------|----------------------|----------------------|----------------------|----------------|
| Two-way | (poutcome = non-exist) \ast month = mar (+) | (poutcome = non-exist) \ast month = oct (+) | (poutcome = non-exist) \ast education = univ (+) | (poutcome = non-exist) \ast contact = telephone (−) | (poutcome = non-exist) \ast housing = unkown (−) |
| Three-way | (job = technician) \ast (education = professional) \ast (marital = married) (+) | (poutcome = non-exist) \ast education = univ \ast (marital = single) (+) |

Table 3: Selected variables with signs of coefficients in parentheses.
A Appendix

A.1 Proof of Theorem 2

The result is an application of Theorem 2.1 of Luo and Tseng (1992). In fact, under the assumptions made in Section 1.2 and the assumption in this theorem, \( g(\mathbf{X}\beta) \triangleq q^T \exp(\mathbf{X}\beta) \) is strictly convex and twice continuously differentiable on its effective domain, and \( \nabla^2 g(\mathbf{X}\beta) \) is positive definite. It follows from Theorem 2.1 of Luo and Tseng (1992) that \( \{\beta(t)\}^{\infty}_{t=0} \) generated by the Algorithm 1 (with cyclic update) converges to \( \hat{\beta} \) at least linearly.

A.2 Proof of Theorem 3

We prove the conclusion by induction. Given \( \ddot{\beta}^{(t)}, \dot{\mu}^{(t)}, \bar{\mu}^{(t)} \) with \( \bar{\mu}^{(t)} = \dot{\mu}^{(t)}/\langle 1, \dot{\mu}^{(t)} \rangle \), it suffices to show that (i) equation (25) and equation (27) yield the same solution, and (ii) \( \bar{\mu}^{(t+1)} \) obtained from (28) and \( \dot{\mu}^{(t+1)} \) updated from (26) satisfy \( \bar{\mu}^{(t+1)} = \dot{\mu}^{(t+1)}/\langle 1, \dot{\mu}^{(t+1)} \rangle \).

Plugging \( \bar{\mu}^{(t)} = \dot{\mu}^{(t)}/\langle 1, \dot{\mu}^{(t)} \rangle \) into (25) gives:

\[
\langle 1, n \rangle \sum_i \ddot{x}_{ij} \dot{\mu}_i^{(t)} \exp[\ddot{x}_{ij}(\ddot{\beta}_j^{(t+1)} - \ddot{\beta}_j^{(t)})] = \sum_i n_i \ddot{x}_{ij},
\]
or equivalently

\[
\sum_i \ddot{x}_{ij} \dot{\mu}_i^{(t)} \exp[\ddot{x}_{ij}(\ddot{\beta}_j^{(t+1)} - \ddot{\beta}_j^{(t)})] = \sum_i (n_i/\langle 1, n \rangle) \ddot{x}_{ij},
\]

which is exactly (27).

Next, given \( \ddot{\beta}^{(t+1)} \), we have

\[
\frac{\bar{\mu}^{(t+1)}}{\langle 1, \dot{\mu}^{(t+1)} \rangle} = \frac{\dot{\mu}^{(t)} \circ \exp[\ddot{X}(\ddot{\beta}^{(t+1)} - \ddot{\beta}^{(t)})]}{\langle 1, \dot{\mu}^{(t)} \circ \exp[\ddot{X}(\ddot{\beta}^{(t+1)} - \ddot{\beta}^{(t)})] \rangle} = \frac{[\dot{\mu}^{(t)}/\langle 1, \dot{\mu}^{(t)} \rangle] \circ \exp[\ddot{X}(\ddot{\beta}^{(t+1)} - \ddot{\beta}^{(t)})]}{\langle 1, [\dot{\mu}^{(t)}/\langle 1, \dot{\mu}^{(t)} \rangle] \circ \exp[\ddot{X}(\ddot{\beta}^{(t+1)} - \ddot{\beta}^{(t)})] \rangle} = \frac{\bar{\mu}^{(t)} \circ \exp[\ddot{X}(\ddot{\beta}^{(t+1)} - \ddot{\beta}^{(t)})]}{\langle 1, \dot{\mu}^{(t)} \circ \exp[\ddot{X}(\ddot{\beta}^{(t+1)} - \ddot{\beta}^{(t)})] \rangle} = \dot{\mu}^{(t+1)},
\]
where the third equality follows from the induction hypothesis, and the last equality is due to (28).

A.3 Proof of Theorem 4

Let $f_1(\beta) = -\langle n, x \rangle \beta + \langle q, \exp(\beta x) \rangle + \lambda \beta$. From the Karush–Kuhn–Tucker equation

$$x^T \mu - x^T n + \lambda s(\beta) = 0,$$

where $\mu = q \circ \exp(\beta x)$ and the sub-gradient $s(\beta)$ satisfies $s(\beta) = \text{sgn}(\beta)$ if $\beta \neq 0$ and $s(\beta) \in [-1, 1]$ if $\beta = 0$. For such a convex problem, this equation is necessary and sufficient for the solution.

Recall (8), and so we have $x^T \mu = \langle x, q \rangle \exp \beta$. Plugging this into (33) gives $\langle x, q \rangle \exp \beta - x^T n + \lambda s(\beta) = 0$. The solution thus follows

$$\hat{\beta} = \begin{cases} 
\log \frac{\langle x, n \rangle - \lambda}{\langle x, q \rangle}, & \text{if } \langle x, n - q \rangle \geq \lambda \\
0, & \text{if } -\lambda < \langle x, n - q \rangle < \lambda \\
\log \frac{\langle x, n \rangle + \lambda}{\langle x, q \rangle}, & \text{if } \langle x, n - q \rangle \leq -\lambda.
\end{cases}$$

In the $\ell_0$ case, let $f_0(\beta) = -\langle n, x \rangle \beta + \langle q, \exp(\beta x) \rangle + \lambda 1_{\beta \neq 0}$ which is nonconvex, and $\hat{\beta}$ a global minimizer of $f_0$. Notice that given a binary vector $x$, we have

$$\exp(\beta x) = \exp(\beta x) + (1 - x),$$

from which it follows that

$$f_0(\beta) = -\langle n, x \rangle \beta + \langle q, x \rangle \exp(\beta) + \langle q, 1 - x \rangle + \lambda 1_{\beta \neq 0}. \quad (34)$$

If $\hat{\beta} \neq 0$, $\partial f_0/\partial \beta = 0$ gives $\hat{\beta} = \log((\langle n, x \rangle)/\langle q, x \rangle)$, where $\langle n, x \rangle \neq \langle q, x \rangle$, and so $f_0(\hat{\beta}) = -\langle n, x \rangle \log((\langle n, x \rangle)/\langle q, x \rangle) + \langle n, x \rangle \log((\langle n, x \rangle)/\langle q, x \rangle) + \lambda 1_{\beta \neq 0}$.

The condition $f_0(\hat{\beta}) \leq f_0(0) = \langle q, 1 \rangle$ can be expressed as

$$-\langle n, x \rangle \log((\langle n, x \rangle)/\langle q, x \rangle) + \langle n, x \rangle - \langle q, x \rangle + \lambda \leq 0,$$

which is equivalent to $D_{KL}((\langle n, x \rangle)/\langle q, x \rangle) \geq \lambda$. In summary, a globally optimal solution of $\min_{\beta \in \mathbb{R}} f_0(\beta)$ is

$$\hat{\beta} = \begin{cases} 
0, & \text{if } D_{KL}((\langle n, x \rangle)/\langle q, x \rangle) < \lambda, \\
\log((\langle n, x \rangle)/\langle q, x \rangle), & \text{if } D_{KL}((\langle n, x \rangle)/\langle q, x \rangle) \geq \lambda.
\end{cases}$$

It is worth mentioning that $\hat{\beta}$ is not unique if $D_{KL}((\langle n, x \rangle)/\langle q, x \rangle) = \lambda$, in which case $\hat{\beta}$ can take either 0 or $\log((\langle n, x \rangle)/\langle q, x \rangle)$. 
A.4 Large experiments

This part tests the performance of B-IPS on large tables and large designs with dimensionality \( p \geq 20000 \). The experiments were performed on a machine with 2.9GHz CPU and 64GB RAM installed. We consider 6 examples. The first three come from contingency tables, consisting of 200, 225 and 250 binary categorical variables, respectively. All interactions (up to second order) are included, resulting in \( p = 20,101, p = 25,426 \), and \( p = 31,376 \), respectively. The observed entries are sampled from the table and the number \( N \) is fixed at 100,000. In generating the coefficients, we let the intercept take 5, and set all \( \beta_j^* \) to zero except the last 100 which are sampled from \( \mathcal{N}(-1, 1) \). The error tolerance \( \epsilon_{\text{tol}} \) in the stopping criterion is 1e-5. The remaining three examples have large design matrices involving non-binary features, where \( N = 100,000 \) and \( p \) varies from 20,000 to 30,000. In these examples, \( \beta_0 = 10 \) and \( \beta_j^* \) are i.i.d. following \( 0.5\mathcal{N}(10, 1) + 0.5\mathcal{N}(-10, 1) \), \( 1 \leq j \leq p - 1 \). The prototype design matrix is scaled, \( \tilde{X} \leftarrow \tilde{X}/(200\|\tilde{X}\|_{\text{max}}) \), and \( \epsilon_{\text{tol}} = 1\text{-e}^{-7} \). The block sizes in calling B-IPS are fixed at 5000 (or approximately so). The computational time and estimation error for are reported in the following table.

Table 4: Computational and statistical performance of B-IPS on large tables and designs, where Time is in seconds, and Err denotes the relative estimation error defined in Section 5.

|       | Ex 1 | Ex 2 | Ex 3 | Ex 4 | Ex 5 | Ex 6 |
|-------|------|------|------|------|------|------|
| \( p \) | 20,101 | 25,426 | 31,376 | 20,000 | 25,000 | 30,000 |
| Time  | 2.9e+4 | 3.5e+4 | 0.24  | 3.9e+4 | 0.33  | 1.8e+3 |
| Err   | 0.039  | 0.24  | 0.33  | 0.0005 | 0.002 | 0.005 |

References

Agresti, A. (2012). *Categorical Data Analysis*. John Wiley & Sons, New York, 3rd edition.

Akaike, H. (1974). A new look at the statistical model identification. *IEEE transactions on automatic control*, 19(6):716–723.
Anna, K. and Tamás, R. (2015). Iterative scaling in curved exponential families. *Scandinavian Journal of Statistics*, 42(3):832–847.

Berger, A. L., Pietra, V. J. D., and Pietra, S. A. D. (1996). A maximum entropy approach to natural language processing. *Comput. Linguist.*, 22(1):39–71.

Bertsekas, D. P. (2015). *Convex Optimization Algorithms*. Athena Scientific, Belmont.

Bishop, Y. M. M., Fienberg, S. E., and Holland, P. W. (1975). *Discrete multivariate analysis: theory and practice*. The MIT Press, Cambridge.

Bohning, D. and Lindsay, B. G. (1988). Monotonicity of quadratic-approximation algorithms. *Annals of the Institute of Statistical Mathematics*, 40(4):641–663.

Boyd, S. and Vandenberghe, L. (2004). *Convex optimization*. Cambridge University Press, New York.

Chen, J. and Chen, Z. (2008). Extended Bayesian information criteria for model selection with large model spaces. *Biometrika*, 95(3):759–771.

Csiszár, I. (1975). I-divergence geometry of probability distributions and minimization problems. *The Annals of Probability*, pages 146–158.

Darroch, J. N. and Ratcliff, D. (1972). Generalized iterative scaling for log-linear models. *The annals of mathematical statistics*, pages 1470–1480.

Deming, W. E. and Stephan, F. F. (1940). On a least squares adjustment of a sampled frequency table when the expected marginal totals are known. *The Annals of Mathematical Statistics*, 11(4):427–444.

Dudík, M., Phillips, S. J., and Schapire, R. E. (2004). *Performance Guarantees for Regularized Maximum Entropy Density Estimation*, pages 472–486. Springer Berlin Heidelberg, Berlin, Heidelberg.

Elith, J., Phillips, S. J., Hastie, T., Dudík, M., Chee, Y. E., and Yates, C. J. (2011). A statistical explanation of maxent for ecologists. *Diversity and Distributions*, 17(1):43–57.
Fienberg, S. E. (1970). An iterative procedure for estimation in contingency tables. *The Annals of Mathematical Statistics*, pages 907–917.

Fienberg, S. E. and Meyer, M. M. (2006). Iterative proportional fitting. *Encyclopedia of Statistical Sciences*, 6:3723–3726.

Fienberg, S. E. and Rinaldo, A. (2012). Maximum likelihood estimation in log-linear models. *Ann. Statist.*, 40(2):996–1023.

Good, I. J. (1963). Maximum entropy for hypothesis formulation, especially for multidimensional contingency tables. *The Annals of Mathematical Statistics*, pages 911–934.

Haberman, S. J. (1974). *The analysis of frequency data*. The University of Chicago Press, Chicago.

Hunter, D. R. and Lange, K. (2004). A tutorial on MM algorithms. *The American Statistician*, 58(1):30–37.

Ireland, C. T. and Kullback, S. (1968). Contingency tables with given marginals. *Biometrika*, 55(1):179–188.

Kurras, S. (2015). Symmetric iterative proportional fitting. In *Proceedings of the Eighteenth International Conference on Artificial Intelligence and Statistics*, pages 526–534.

Lahr, M. and De Mesnard, L. (2004). Biproportional techniques in input-output analysis: table updating and structural analysis. *Economic Systems Research*, 16(2):115–134.

Lange, K. (2013). *Optimization*. Springer, New York, 2nd edition.

Lange, K., Hunter, D. R., and Yang, I. (2000). Optimization transfer using surrogate objective functions. *Journal of computational and graphical statistics*, 9(1):1–20.

Lauritzen, S. L. (1996). *Graphical models*. Oxford University Press, New York.

Liu, D. C. and Nocedal, J. (1989). On the limited memory BFGS method for large scale optimization. *Mathematical programming*, 45(1-3):503–528.
Luo, Z.-Q. and Tseng, P. (1992). On the convergence of the coordinate descent method for convex differentiable minimization. *Journal of Optimization Theory and Applications*, 72(1):7–35.

McCallum, A., Freitag, D., and Pereira, F. C. N. (2000). Maximum entropy Markov models for information extraction and segmentation. In *Proceedings of the 7th International Conference on Machine Learning*.

Moro, S., Cortez, P., and Rita, P. (2014). A data-driven approach to predict the success of bank telemarketing. *Decision Support Systems*, 62:22–31.

Nesterov, Y. (1988). On an approach to the construction of optimal methods of minimization of smooth convex functions. *Ekonomika i Matem Metody*, 24(3):509–517.

Nesterov, Y. (2012). Efficiency of coordinate descent methods on huge-scale optimization problems. *SIAM Journal on Optimization*, 22(2):341–362.

Nutini, J., Schmidt, M., Laradji, I. H., Friedlander, M., and Koepke, H. (2015). Coordinate descent converges faster with the Gauss-Southwell rule than random selection. In *Proceedings of the 32nd International Conference on Machine Learning (ICML-15)*, pages 1632–1641.

Phillips, S. J., Dudík, M., and Schapire, R. E. (2004). A maximum entropy approach to species distribution modeling. In *Proceedings of the 21th International Conference on Machine Learning*.

Pietra, S. D., Pietra, V. D., and Lafferty, J. (1997). Inducing features of random fields. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 19(4):380–393.

Pukelsheim, F. (2014). Biproportional scaling of matrices and the iterative proportional fitting procedure. *Annals of Operations Research*, 215(1):269–283.

Razaviyayn, M., Hong, M., and Luo, Z.-Q. (2013). A unified convergence analysis of block successive minimization methods for nonsmooth optimization. *SIAM Journal on Optimization*, 23(2):1126–1153.

Richtárik, P. and Takáč, M. (2014). Iteration complexity of randomized block-coordinate descent methods for minimizing a composite function. *Mathematical Programming*, 144(1-2):1–38.
Schmidt, M. (2012). minFunc: unconstrained differentiable multivariate optimization in Matlab. http://www.cs.ubc.ca/~schmidtm/Software/minFunc.html.

Sinkhorn, R. (1964). A relationship between arbitrary positive matrices and doubly stochastic matrices. The Annals of Mathematical Statistics, 35(2):876–879.

Sinkhorn, R. and Knopp, P. (1967). Concerning nonnegative matrices and doubly stochastic matrices. Pacific Journal of Mathematics, 21(2):343–348.

Tseng, P. (2001). Convergence of a block coordinate descent method for nondifferentiable minimization. Journal of optimization theory and applications, 109(3):475–494.

Tseng, P. (2010). Approximation accuracy, gradient methods, and error bound for structured convex optimization. Mathematical Programming, 125(2):263–295.

Wang, N., Rauh, J., and Massam, H. (2016). Approximating faces of marginal polytopes in discrete hierarchical models. arXiv preprint arXiv:1603.04843.

Wright, S. J. (2015). Coordinate descent algorithms. Mathematical Programming, 151(1):3–34.