Asymptotic Convergence Properties of EM-Type Algorithms[1]

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ABSTRACT

We analyze the asymptotic convergence properties of a general class of EM-type algorithms for estimating an unknown parameter via alternating estimation and maximization. As examples, this class includes ML-EM, penalized ML-EM, Green's OSL-EM, and many other approximate EM algorithms. A theorem is given which provides conditions for monotone convergence with respect to a given norm and specifies an asymptotic rate of convergence for an algorithm in this class. By investigating different parameterizations, the condition for monotone convergence can be used to establish norms under which the distance between successive iterates and the limit point of the EM-type algorithm approaches zero monotonically. We apply these results to a modified ML-EM algorithm with stochastic complete/incomplete data mapping and establish global monotone convergence for a linear Gaussian observation model. We then establish that in the final iterations the unpenalized and quadratically penalized ML-EM algorithms for PET image reconstruction converge monotonically relative to two different norms on the logarithm of the images.

I. INTRODUCTION

The maximum-likelihood (ML) expectation-maximization (EM) algorithm is a popular iterative method for finding the maximum likelihood estimate $\hat{\theta}$ of a parameter θ when the likelihood function is too difficult to maximize directly [4, 23, 17, 18, 19, 5, 22]. The penalized ML-EM algorithm is a variant of the ML-EM algorithm which can be used for finding MAP estimates of a random parameter [10, 11, 12]. To apply the penalized or unpenalized ML-EM algorithm requires formulation of the estimation problem in terms of the actual data sample, called the *incomplete data*, and a hypothetical data set, called the *complete data*. To be able to easily implement the ML-EM algorithm the complete data must be chosen in such a way that: the complete data log-likelihood function is easily estimated from the incomplete data via conditional expectation (E); and the complete data log-likelihood function is easily maximized (M). Three types of convergence results are of practical importance: conditions under which the sequence of estimates converges globally to a

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fixed point, norms under which the convergence is monotone; and the asymptotic convergence rate of the algorithm. A number of authors [24, 16, 3] have derived global convergence results for a wide range of exact ML-EM algorithms by using an information divergence approach. These authors establish monotone convergence of ML-EM algorithms in the information divergence measure. This guarantees that successive iterates of the EM algorithm monotonically increase likelihood. While increasing likelihood is an attractive property, it does not guarantee monotone convergence in terms of Cauchy convergence: successive iterates of the EM algorithm reduce the distance to the ML estimate in some norm. In addition, for some implementations the region of convergence may only be a small subset of the entire parameter space so that global convergence may not hold. Furthermore, in some cases the ML-EM algorithm can only be implemented by making simplifying approximations in the conditional expectation step (E) or the maximization step (M). While these algorithms have an alternating estimation-maximization structure similar to the exact ML-EM algorithm, the information divergence approach developed to establish global convergence of the exact ML-EM algorithm may not be effective. In this paper we develop a generally applicable approach to convergence analysis which allows us to study monotone convergence and asymptotic convergence rates for algorithms which can be implemented via alternating estimation-maximization.

We define an EM-type algorithm as any iterative algorithm of the form $\theta^{i+1} = \mathbf{argmax}_\theta\, Q(\theta, \theta^i)$, $i = 1, 2, \ldots$ where $\theta \in \Theta \subset \mathbb{R}^p$. This general iterative algorithm specializes to popular EM-type algorithms including: penalized and penalized ML-EM algorithms [4, 11], generalized ML-EM with stochastic complete-incomplete data mapping [6], one-step-late (OSL) penalized ML-EM [9], majorization methods [**?**], and approximate ML-EM algorithms such as the linear and quadratic approximations introduced in [2, 1]. Let θ^* be a fixed point of the EM-type algorithm which occurs on the interior of Θ and assume that Q is a smooth function of both arguments. We give an implicit relation between successive differences $\Delta\theta^{i+1} \stackrel{\text{def}}{=} \theta^{i+1} - \theta^*$ and $\Delta\theta^i \stackrel{\text{def}}{=} \theta^i - \theta^*$ of the form $\Delta\theta^{i+1} = M_1^{-1} M_2 \Delta\theta^{i+1}$ where M_1 and M_2 are $p \times p$ matrices associated with the $2p \times 2p$ Hessian matrix of $Q(\theta^{i+1}, \theta^i)$. Using this implicit relation we derive conditions for monotone convergence and show that the asymptotic rate of convergence is the maximum magnitude eigenvalue of the curvature matrix $[\nabla^{20} Q(\theta^*, \theta^*)]^{-1} \nabla^{11} Q(\theta^*, \theta^*)$ where $\nabla^{20} Q$ and $\nabla^{11} Q$ are $p \times p$ matrices of mixed derivatives at the point (θ^*, θ^*). For ML-EM this curvature matrix is monotonically increasing in the conditional Fisher information matrix associated with the complete data.

We provide several illustrations of our convergence results. First we consider a generalized version of the standard ML-EM algorithm which permits the complete data to be specified in such a way that it is related to the incomplete data via a possibly *random* transformation. This algorithm is of interest since the conventional convergence analysis of the EM algorithm is inapplicable due to the presence of additive noise in the mapping from the complete data to the incomplete data. Then we give general forms for the asymptotic convergence rates for the linearized EM algorithm [2], the unpenalized and penalized ML-EM algorithms, the OSL penalized ML-EM algorithm [9], and the majorization method [**?**]. For the latter algorithms the asymptotic convergence rates are of similar form to those obtained by Green [9] for the standard case of deterministic complete/incomplete data mapping. Afterwards we consider ML-EM and penalized ML-EM for two important practical examples: a linear model involving jointly Gaussian statistics for the complete and incomplete data and a PET reconstruction model involving jointly Poisson statistics. For the linear Gaussian model the incomplete data is the output of a Gaussian additive noise channel with input equal to the complete data. We show that it is necessary for the channel noise to be uncorrelated with the channel input, i.e. the complete data set, in order to guarantee convergence to the ML estimate. It is found that the ML-EM algorithm is guaranteed to converge monotonically in a weighted Euclidean norm for all initial points and is therefore globally monotonically convergent in this norm. It is also found that increasing the channel noise variance can only degrade the asymptotic convergence rate of the ML-EM algorithm. For the PET reconstruction model we show that when the unpenalized ML-EM algorithm converges to a strictly positive estimate, in the final iterations convergence is monotone in the following sense: the logarithm $\ln \theta^i$ of the i-th image converges monotonically in the weighted Euclidean norm $\|u\| = \sum_{b=1}^p P_b \hat{\theta}_b\, u^2$, where P_b is the probability of detecting emissions at pixel b and $\hat{\theta}$ is the ML estimate. When $P_b \equiv 1$, this is asymptotically equivalent to monotone convergence of the error ratios $\left[\frac{\Delta\theta_1^i}{\theta_1^*}, \ldots, \frac{\Delta\theta_p^i}{\theta_p^*}\right]^T$ to zero in the standard unweighted Euclidean norm. Similar results are obtained for quadratically penalized ML-EM algorithms for PET reconstruction.

II. AN ARCHETYPE ALGORITHM

Let $\theta = [\theta_1, \ldots, \theta_p]^T$ be a real parameter residing in an open subset $\Theta = \Theta_1 \times \cdots \times \Theta_p$ of the p-dimensional space $\mathbb{R}^p$. Given a function $Q : \Theta \times \Theta \to \mathbb{R}$ and an intial point $\theta^0 \in \Theta$, consider the following recursive algorithm, called the A-algorithm:

$$\textbf{A-Algorithm:} \qquad \theta^{i+1} = \mathop{\mathbf{argmax}}_{\theta\in\Theta} Q(\theta, \theta^i), \qquad i = 0, 1, \ldots. \tag{1}$$

(If there are multiple maxima, then θ^{i+1} can be taken to be any one of them.) Assume that $\theta^* \in \Theta$ is a fixed point of the recursive mapping (1), i.e. θ^* satisfies:

$$\theta^* = \mathop{\mathbf{argmax}}_{\theta\in\Theta} Q(\theta, \theta^*). \tag{2}$$

Let $\|\cdot\|$ denote a vector norm on $\mathbb{R}^p$. For any $p \times p$ matrix $\mathbf{A}$ the induced *matrix norm* $|||\mathbf{A}|||$ [13] of $\mathbf{A}$ is defined as:

$$|||\mathbf{A}||| \stackrel{\text{def}}{=} \max_{u\in\mathbb{R}^p} \frac{\|\mathbf{A}u\|}{\|u\|}, \tag{3}$$

where u denotes a vector in $\mathbb{R}^p$. A special case is the *matrix-2* norm $|||\mathbf{A}|||_2$ which is induced by the Euclidean vector norm $\|u\| = u^T u$:

$$|||\mathbf{A}|||_2 \stackrel{\text{def}}{=} \sqrt{\max_u \frac{u^T \mathbf{A}^T \mathbf{A} u}{u^T u}}..$$

$\|\mathbf{A}\|_2^2$ is the maximum eigenvalue of $\mathbf{A}^T\mathbf{A}$. We say that a sequence u^i, $i = 1, 2, \ldots$, converges monotonically to a point u^* in the norm $\|\cdot\|$ if:

$$\|u^{i+1} - u^*\| < \|u^i - u^*\|, \qquad i = 1, 2, \ldots. \tag{4}$$

Consider the general linear iteration of the form

$$v^{i+1} = \mathbf{A} v^i, \qquad i = 1, 2, \ldots$$

with $\|\mathbf{A}\| < 1$. Then, since $\|v^{i+1}\| \leq \|\mathbf{A}\| \cdot \|v^i\| < \|v^i\|$, the sequence $\{v^i\}$ converges monotonically to zero and the asymptotic rate of convergence is specified by the *root convergence factor* $\rho(\mathbf{A})$ which is defined as the largest magnitude eigenvalue of $\mathbf{A}$ [20]. Observe that $\rho(\mathbf{A})$ is identical to $\|\mathbf{A}\|_2$ if $\mathbf{A}$ is real symmetric non-negative definite.

Assume that the function $Q(\theta, \overline{\theta})$ is twice continuously differentiable in both arguments θ and $\overline{\theta}$ over $\theta, \overline{\theta} \in \Theta$. We define the Hessian matrix of Q over $\Theta \times \Theta$ as the following block partioned $2p \times 2p$ matrix:

$$\nabla^2 Q(\theta, \overline{\theta}) = \begin{bmatrix} \nabla^{20} Q(\theta, \overline{\theta}) & \nabla^{11} Q(\theta, \overline{\theta}) \\ \nabla^{11} Q(\theta, \overline{\theta}) & \nabla^{02} Q(\theta, \overline{\theta}) \end{bmatrix}, \tag{5}$$

where $\nabla^{20} Q(\theta, \overline{\theta}) = \nabla_\theta \nabla_\theta^T Q(\theta, \overline{\theta})$, $\nabla^{02} Q(\theta, \overline{\theta}) = \nabla_{\overline{\theta}} \nabla_{\overline{\theta}}^T Q(\theta, \overline{\theta})$, and $\nabla^{11} Q(\theta, \overline{\theta}) = \nabla_{\overline{\theta}} \nabla_\theta^T Q(\theta, \overline{\theta})$ are $p \times p$ matrices of partial derivatives $\frac{\partial^2}{\partial\theta_i \partial\theta_j} Q(\theta, \overline{\theta})$, $\frac{\partial^2}{\partial\overline{\theta}_i \partial\overline{\theta}_j} Q(\theta, \overline{\theta})$, and $\frac{\partial^2}{\partial\overline{\theta}_i \partial\theta_j} Q(\theta, \overline{\theta})$, $i, j = 1, \ldots, p$, respectively.

A *region of monotone convergence* relative to the vector norm $\|\cdot\|$ of the A-algorithm (1) is defined as any open ball $B(\theta^*, \delta) = \{\theta : \|\theta - \theta^*\| \leq \delta\}$ centered at $\theta = \theta^*$ with radius $\delta > 0$ such that if the initial point θ^0 is in this region then $\|\theta^i - \theta^*\|$, $i = 1, 2, \ldots$, converges monotonically to zero. Note that as defined, the shape in $\mathbb{R}^p$ of the region of monotone convergence depends on the norm used. For the Euclidean norm $\|u\| = u^T u$ the region of monotone convergence is a spherically shaped region in Θ. For a general positive definite matrix $\mathbf{B}$ the induced norm $\|u\| = u^T B u$ makes this region an ellipsoid in Θ. Since all norms are equivalent for the case of a finite dimensional parameter space, monotone convergence in a given norm implies convergence, however possibly non-monotone, in any other norm.

Define the $p \times p$ matrices obtained by averaging $\nabla^{20} Q(u, \overline{u})$ and $\nabla^{11} Q(u, \overline{u})$ over the line segments $u \in \vec{\theta\theta^*}$ and $\overline{u} \in \vec{\overline{\theta}\theta^*}$:

$$\tag{6}$$

$$\begin{aligned} A_1(\theta, \overline{\theta}) &= -\int_0^1 \nabla^{20} Q(t\theta + (1-t)\theta^*, t\overline{\theta} + (1-t)\theta^*) dt \\ A_2(\theta, \overline{\theta}) &= \int_0^1 \nabla^{11} Q(t\theta + (1-t)\theta^*, t\overline{\theta} + (1-t)\theta^*) dt. \end{aligned}$$

For $t_k \in [0,1]$, $k = 1, \ldots, p$, define the $p \times p$ matrices obtained by taking each of the p rows of $\nabla^{20} Q(\theta, \overline{\theta})$ and $\nabla^{11} Q(\theta, \overline{\theta})$ and replacing θ and $\overline{\theta}$ with points $\theta(t_k) \stackrel{\text{def}}{=} t_k\theta + (1-t_k)\theta^*$ and $\overline{\theta}(t_k) \stackrel{\text{def}}{=} t_k\overline{\theta} + (1-t_k)\theta^*$:

$$
\mathcal{A}_1(\theta, \overline{\theta}) = -\begin{bmatrix} \nabla_\theta \frac{\partial}{\theta_1} Q(\theta, \overline{\theta}(t_1))|_{\theta=\theta(t_1)} \\ \vdots \\ \nabla_\theta \frac{\partial}{\theta_p} Q(\theta, \overline{\theta}(t_p))|_{\theta=\theta(t_p)} \end{bmatrix}
$$

$$
\mathcal{A}_2(\theta, \overline{\theta}) = \begin{bmatrix} \nabla_{\overline{\theta}} \frac{\partial}{\theta_1} Q(\theta, \overline{\theta})|_{\theta=\theta(t_1), \overline{\theta}=\overline{\theta}(t_1)} \\ \vdots \\ \nabla_{\overline{\theta}} \frac{\partial}{\theta_p} Q(\theta, \overline{\theta})|_{\theta=\theta(t_p), \overline{\theta}=\overline{\theta}(t_p)} \end{bmatrix}. \tag{7}
$$

Definition 1 *For M_1 and M_2 defined as either A_1 and A_1 in (6) or as $\mathcal{A}_1$ and $\mathcal{A}_2$ in (7), define $\mathcal{R}_+ \subset \Theta$ as the largest open ball $B(\theta^*, \delta) = \{\theta : \|\theta - \theta^*\| \leq \delta\}$ such that for each $\overline{\theta} \in B(\theta^*, \delta)$:*

$$
M_1(\theta, \overline{\theta}) > 0, \qquad \text{for all } \theta \in \Theta \tag{8}
$$

and for some $0 \leq \alpha^2 < 1$

$$
\left\| \left[M_1(\theta, \overline{\theta}) \right]^{-1} \cdot M_2(\theta, \overline{\theta}) \right\| \leq \alpha^2, \qquad \text{for all } \theta \in \Theta. \tag{9}
$$

The following convergence theorem establishes that, if $\mathcal{R}_+$ is not empty, the region in Definition 1 is a region of monotone convergence in the norm $\|\cdot\|$ for an algorithm of the form (1).

Theorem 1 *Let $\theta^* \in \Theta$ be a fixed point of the A algorithm (1) $\theta^{i+1} = \mathbf{argmax}_{\theta \in \Theta} Q(\theta, \theta^i)$, $i = 0, 1, \ldots$. Assume: i) for all $\overline{\theta} \in \Theta$, the maximum $\max_\theta Q(\theta, \overline{\theta})$ is achieved on the interior of the set Θ; ii) $Q(\theta, \overline{\theta})$ is twice continuously differentiable in $\theta \in \Theta$ and $\overline{\theta} \in \Theta$. Let the point θ^0 initialize the A algorithm.*

1. *If the positive definiteness conditions (8) is satisfied, then the sucessive differences $\Delta\theta^i = \theta^i - \theta^*$ of the A algorithm obey the recursion:*

$$
\Delta\theta^{i+1} = [M_1(\theta^{i+1}, \theta^i)]^{-1} M_2(\theta^{i+1}, \theta^i) \cdot \Delta\theta^i, \qquad i = 0, 1, \ldots, \tag{10}
$$

2. *If $\theta^0 \in \mathcal{R}_+$ for a norm $\|\cdot\|$, then $\|\Delta\theta^i\|$ converges monotonically to zero with at least linear rate, and*

3. $\Delta\theta^i$ asymptotically converges to zero with root convergence factor

$$\rho\left(\left[-\nabla^{20}Q(\theta^*,\theta^*)\right]^{-1}\nabla^{11}Q(\theta^*,\theta^*)\right) < 1.$$

Proof of Theorem 1:

Define $\Delta\theta = \theta - \theta^*$ and $\Delta\theta^i = \theta^i - \theta^*$. Convergence will be established by showing that $\|\Delta\theta^{i+1}\| < \|\Delta\theta^i\|$. Define the $2p\times 1$ vectors $\xi = \begin{bmatrix}\theta\\ \theta^i\end{bmatrix}$, $\xi^* = \begin{bmatrix}\theta^*\\ \theta^*\end{bmatrix}$ and $\Delta\xi = \xi - \xi^*$. By assumption ii we can use the Taylor formula with remainder [21, Eq. B.1.4] to expand $Q_{10}(\xi) \stackrel{\text{def}}{=} [\nabla^{10}Q(\theta,\theta^i)]^T$ about the point $\xi = \xi^* = \begin{bmatrix}\theta^*\\ \theta^*\end{bmatrix}$:

$$Q_{10}(\xi) \;=\; Q_{10}(\xi^*) + \int_0^1 \nabla_\xi Q_{10}(t\xi + (1-t)\xi^*)dt\;\Delta\xi.$$

Now since by assumption i, $\theta^* = \mathbf{argmax}_{\theta\in\Theta}\,Q(\theta,\theta^*)$ occurs in the interior of Θ: $Q_{10}(\xi^*) = \nabla^{10}Q(\theta^*,\theta^*) = 0$, a row vector of zeros. Therefore:

$$Q_{10}(\xi) \;=\; \int_0^1 \nabla_\xi Q_{10}(t\xi + (1-t)\xi^*)\;\Delta\xi dt. \tag{11}$$

¿From definition (6):

$$\int_0^1 \nabla Q_{10}(t\xi + (1-t)\xi^*)dt = \left[\begin{array}{ccc} -A_1(\theta,\theta^i) & \vdots & A_2(\theta,\theta^i)\end{array}\right],$$

we have from (11)

$$\nabla^{10}Q(\theta,\theta^i) = -A_1(\theta,\theta^i)\Delta\theta + A_2(\theta,\theta^i)\Delta\theta^i. \tag{12}$$

On the other hand, consider the k-th element of the left hand side of the (11) and define $\theta(t) = t\theta + (1-t)\theta^*$. From the mean value theorem:

$$\begin{aligned}
&\int_0^1 \left[\nabla_\theta \frac{\partial}{\partial\theta_k}Q(\theta(t),\theta^i(t))\Delta\theta + \nabla_{\theta^i}\frac{\partial}{\partial\theta_k}Q(\theta(t),\theta^i(t))\Delta\theta^i\right]dt\\
&\quad = \nabla_\theta\frac{\partial}{\partial\theta_k}Q(\theta(t_k),\theta^i(t_k))\Delta\theta + \nabla_{\theta^i}\frac{\partial}{\partial\theta_k}Q(\theta(t_k),\theta^i(t_k))\Delta\theta^i\\
&\quad = -[\mathcal{A}_1]_{k*}(\theta,\theta^i)\Delta\theta + [\mathcal{A}_2]_{k*}(\theta,\theta^i)\Delta\theta^i
\end{aligned}$$

where t_k is some point in $[0,1]$, which in general depends on θ, θ^i, and θ^*, and $[\mathcal{A}_1]_{k*}$, $[\mathcal{A}_2]_{k*}$ denote the k-th rows of the matrices $\mathcal{A}_1$, $\mathcal{A}_2$ defined in (7). Therefore (11) is equivalent to

$$\nabla^{10}Q(\theta,\theta^i) = -\mathcal{A}_1(\theta,\theta^i)\Delta\theta + \mathcal{A}_2(\theta,\theta^i)\Delta\theta^i. \tag{13}$$

Combining (12) and (13) we obtain the general relation:

$$\nabla^{10} Q(\theta, \theta^i) = -M_1(\theta, \theta^i)\Delta\theta + M_2(\theta, \theta^i)\Delta\theta^i. \tag{14}$$

where M_1 and M_2 are either A_1 and A_2 or $\mathcal{A}_1$ and $\mathcal{A}_2$. Now, we know $\theta^{i+1} = \mathbf{argmax}_\theta\, Q(\theta, \theta^i)$ lies in the interior of Θ, $\nabla^{10} Q(\theta^{i+1}, \theta^i) = 0$. Therefore from Eq. (14):

$$-M_1(\theta^{i+1}, \theta^i)\Delta\theta^{i+1} + M_2(\theta^{i+1}, \theta^i)\Delta\theta^i = 0. \tag{15}$$

Now if the positivity condition (8) holds for $\overline{\theta} = \theta^i$ then $M_1(\theta, \theta^i)$ is invertible for all θ and it follows from Eq. (15) that:

$$\Delta\theta^{i+1} = [M_1(\theta^{i+1}, \theta^i)]^{-1} M_2(\theta^{i+1}, \theta^i) \cdot \Delta\theta^i, \tag{16}$$

Furthermore, by properties of matrix norms [7]:

$$\begin{aligned} \|\Delta\theta^{i+1}\| &\leq \left\|\!\left| M_1(\theta^{i+1}, \theta^i)]^{-1} M_2(\theta^{i+1}, \theta^i) \right|\!\right\| \cdot \|\Delta\theta^i\| \\ &\leq \sup_{\theta \in \Theta} \left\|\!\left| [M_1(\theta, \theta^i)]^{-1} M_2(\theta, \theta^i) \right|\!\right\| \cdot \|\Delta\theta^i\|. \end{aligned} \tag{17}$$

Therefore, if $\theta^i \in \mathcal{R}_+$, by condition (9) $\sup_{\theta\in\Theta} \left\|\!\left| [M_1(\theta, \theta^i)]^{-1} M_2(\theta, \theta^i) \right|\!\right\| \leq \alpha^2 < 1$ so that:

$$\|\Delta\theta^{i+1}\| \quad \leq \quad \alpha^2 \cdot \|\Delta\theta^i\|.$$

Since $\mathcal{R}_+$ is an open ball centered at θ^* which contains θ^i, this implies that $\theta^{i+1} \in \mathcal{R}_+$. By induction on i we conclude that $\|\theta^i - \theta^*\|$ converges monotonically to zero with at least linear convergence rate.

Next we establish the asymptotic convergence rate stated in the theorem. By continuity of the derivatives of $Q(\theta, \theta^i)$ and the result (17) we obtain:

$$M_1(\theta^{i+1}, \theta^i) \quad = \quad -\nabla^{20} Q(\theta^*, \theta^*) + O(\|\Delta\theta^i\|)$$

$$M_2(\theta^{i+1}, \theta^i) \quad = \quad \nabla^{11} Q(\theta^*, \theta^*) + O(\|\Delta\theta^i\|).$$

Thus, by continuity of the matrix norm:

$$\alpha^2 \geq \sup_{\theta\in\Theta} \left\|\!\left| [M_1(\theta, \theta^i)]^{-1} M_2(\theta, \theta^i) \right|\!\right\| \quad = \quad \left\|\!\left| \left[-\nabla^{20} Q(\theta^*, \theta^*)\right]^{-1} \nabla^{11} Q(\theta^*, \theta^*) \right|\!\right\| + O(\|\Delta\theta^i\|). \tag{18}$$

Since $\alpha^2 < 1$ taking the limit of (18) as $i \to \infty$ establishes that

$$\left\|\!\left| \left[-\nabla^{20} Q(\theta^*, \theta^*)\right]^{-1} \nabla^{11} Q(\theta^*, \theta^*) \right|\!\right\| < 1. \tag{19}$$

Furthermore (16) takes the asymptotic form:

$$\Delta\theta^{i+1} \quad = \quad -[\nabla^{20} Q(\theta^*, \theta^*)]^{-1} \nabla^{11} Q(\theta^*, \theta^*) \cdot \Delta\theta^i + o(\|\Delta\theta^i\|).$$

Therefore the asymptotic rate of convergence is given by the root convergence factor

$$\rho\left([-\nabla^{20}Q(\theta^*,\theta^*)]^{-1}\nabla^{11}Q(\theta^*,\theta^*)\right).$$

For any matrix $\mathbf{A}$ we have $\rho(\mathbf{A}) \leq |||\mathbf{A}|||$ [13, Thm. 5.6.9] so that, in view of (19), the root convergence factor is less than one. $\square$

The careful reader will have noticed that in the proof of Theorem 1 all that was required of θ^{i+1} was that $\nabla^{10}Q(\theta^{i+1},\theta^i) = 0$. Analogously to the A-algorithm (1) let $\{\theta^i\}$ be a sequence of points in Θ generated by the following *stationary point version* of this algorithm which we call the AZ algorithm:

$$\theta^{i+1} = \text{argzero}_\theta \nabla^{10}Q(\theta,\theta^i), \qquad i = 1,2,\ldots, \tag{20}$$

where $\text{argzero}_\theta\nabla^{10}Q(\theta,\theta^i)$ is any point θ in Θ where the gradient $\nabla^{10}Q(\theta,\theta^i)$ is zero. Note that the stationary point need not be unique; any stationary point will do. If we assume that the algorithm (20) is implementable, i.e. a stationary point exists at each iteration $i = 1,2,\ldots$, then we have:

Corollary 1 *Let $\theta^* \in \Theta$ be a fixed point of the algorithm (1) $\theta^{i+1} = \mathbf{argmax}_{\theta\in\Theta}\, Q(\theta,\theta^i)$, $i = 0,1,\ldots$. Assume: i) for all $\overline{\theta} \in \Theta$, the maximum $\max_\theta Q(\theta,\overline{\theta})$ is achieved on the interior of the set Θ; ii) $Q(\theta,\overline{\theta})$ is twice continuously differentiable in $\theta \in \Theta$ and $\overline{\theta} \in \Theta$; iii) relative to the matrix norm $|||\cdot|||$ the region of monotone convergence $\mathcal{R}_+$ is non-empty. Let the point θ^0 initialize the AZ algorithm (20). Then Assertions 1 and 2 of Theorem 1 hold for the AZ sequence $\{\theta^i\}$.*

In the case that the parameter space $\Theta = \mathbb{R}^p$ the AZ algorithm (20) is always implementable.

Lemma 1 *In addition to the conditions of Corollary 1 assume that $\Theta = \mathbb{R}^p$. Then for each iteration $i = 1,2,\ldots$ of the AZ algorithm (20) there exists a point θ for which $\nabla^{10}Q(\theta,\theta^i) = 0$.*

Proof

As in the proof of Theorem 1, assuming $\theta^i \in \mathcal{R}_+$ we have from Eq. (12):

$$\begin{aligned}\nabla^{10}Q(\theta,\theta^i) &= -M_1(\theta,\theta^i)\Delta\theta + M_2(\theta,\theta^i)\Delta\theta^i \\ &= -M_1(\theta,\theta^i)\left[\Delta\theta - [M_1(\theta,\theta^i)]^{-1}M_2(\theta,\theta^i)\cdot\Delta\theta^i\right] \\ &= -M_1(\theta,\theta^i)\cdot d(\theta)\end{aligned} \tag{21}$$

Where the p-element vector $d(\theta) = \theta - \theta^* - [M_1(\theta,\theta^i)]^{-1}M_2(\theta,\theta^i)\cdot(\theta^i - \theta^*)$ is a function of θ. Since $\rho\left(M_1^{-1}M_2\right) \leq |||M_1^{-1}M_2||| < 1$ for all $\theta \in \Theta$, the eigenvalues of $[M_1]^{-1}M_2$ lie in the interval $(-1,1)$

for all $\theta \in \Theta$. Since $\Theta = \mathbb{R}^p$ is unbounded, there exist points $\theta = \theta_+$ and $\theta = \theta_-$ in Θ such that all p entries of the vector $d(\theta)$ are strictly positive and strictly negative, respectively. Since $d(\theta)$ is continuous this implies that there exists a point $\theta \in \Theta$ such that $d(\theta) = 0$ which implies that $\nabla^{10} Q(\theta, \theta^i) = 0$ as claimed. $\square$

In investigating monotonic convergence properties of the sequence $\{\theta^i\}$ it is sometimes useful to make a transformation of parameters $\theta \to \tau$. Consider a smooth invertible functional transformation g: $\tau = g(\theta)$. Then θ^i can be represented as $g^{-1}(\tau^i)$, where g^{-1} is the inverse of g, the sequence $\{\tau^i\}$ is generated by the analogous A-algorithm:

$$\tau^{i+1} = \mathop{\mathbf{argmax}}_{\tau \in g(\Theta)} \tilde{Q}(\tau, \tau^i), \qquad i = 0, 1, \ldots,$$

and

$$\begin{aligned} \tilde{Q}(\tau, \tau^i) &\stackrel{\text{def}}{=} Q\left(g^{-1}(\tau), g^{-1}(\tau^i)\right) \\ &= Q(\theta, \theta^i)\big|_{\theta = g^{-1}(\tau), \theta^i = g^{-1}(\tau^i)}. \end{aligned}$$

The convergence properties of the sequence $\tau^i = g(\theta^i)$ can be studied using Theorem 1 with M_1 and M_2 defined in terms of the mixed partial derivatives of $\tilde{Q}$:

$$\begin{aligned} \nabla^{11} \tilde{Q}(\tau, \tau^i) &= J^{-1}(\tau) \left[\nabla^{11} Q\left(g^{-1}(\tau), g^{-1}(\tau^i)\right)\right] J^{-1}(\tau^i) \\ \nabla^{20} \tilde{Q}(\tau, \tau^i) &= J^{-1}(\tau) \left[\nabla^{20} Q\left(g^{-1}(\tau), g^{-1}(\tau^i)\right)\right] J^{-1}(\tau). \end{aligned}$$

where $J(\tau) = \nabla g(\theta)|_{\theta = g^{-1}(\tau)}$ is the $p \times p$ Jacobian matrix of partial derivatives of g.

In particular, the relation (10) of Theorem 1 with $M_1 = \mathcal{A}_1$ and $M_2 = \mathcal{A}_2$ gives a recursion for $\Delta\tau^i = g(\theta^i) - g(\theta^*)$:

$$\begin{aligned} \Delta\tau^{i+1} &= [\tilde{\mathcal{A}}_1(\tau^{i+1}, \tau^i)]^{-1} \tilde{\mathcal{A}}_2(\tau^{i+1}, \tau^i) \cdot \Delta\tau^i \qquad (22) \\ &= J(\tau^{i+1}) \left[\mathcal{A}_1\left(g^{-1}(\tau^{i+1}), g^{-1}(\tau^i)\right)\right]^{-1} \mathcal{A}_2(g^{-1}(\tau^{i+1}), g^{-1}(\tau^i)) J^{-1}(\tau^i) \cdot \Delta\tau^i. \end{aligned}$$

III. CONVERGENCE OF THE EM ALGORITHM

Let an observed random variable $\mathbf{Y}$ take values $\{\mathbf{y}\}$ in a set $\mathcal{Y}$ and let $\mathbf{Y}$ have the probability density function $f(\mathbf{y}; \theta)$ where: $\theta = [\theta_1, \ldots, \theta_p]^T$ is a real, non-random parameter vector residing in an open subset $\Theta = \Theta_1 \times \cdots \times \Theta_p$ of the p-dimensional space $\mathbb{R}^p$. Given a realization $\mathbf{Y} = \mathbf{y}$, the penalized maximum likelihood estimator is defined as the parameter value which maximizes the penalized likelihood of the event $\mathbf{Y} = \mathbf{y}$:

$$\hat{\theta} \stackrel{\text{def}}{=} \mathop{\mathbf{argmax}}_{\theta \in \Theta} \{L(\theta) - P(\theta)\} \qquad (23)$$

where $L(\theta) = \ln f(\mathbf{y}; \theta)$ is the log-likelihood function and $P(\theta)$ is a penalty function. If $f(\theta)$ is a prior density for θ, the penalized ML estimator is equivalent to the MAP estimator when $P(\theta) = -\ln f(\theta)$. When $P(\theta)$ is constant we obtain the standard unpenalized ML estimator:

$$\hat{\theta} \stackrel{\text{def}}{=} \mathop{\mathbf{argmax}}_{\theta \in \Theta} \; L(\theta). \tag{24}$$

Under broad conditions the penalized ML estimator enjoys many attractive properties such as consistency, asymptotic unbiasedness, and asymptotic minimum variance among unbiased estimators [14]. However, in many applications direct maximization of the functions in (24) and (23) is intractible. In this case the EM approach offers a simple indirect method for iteratively approximating the penalized and unpenalized ML estimates.

III.a: A General Class of EM Algorithms with Stochastic Mapping

The key to the ML-EM algorithm is to identify $\mathbf{Y}$ as an *incomplete data set* derived from a more informative hypothetical *complete data set* $\mathbf{X}$, where by more informative we mean that $\mathbf{Y}$ can be represented as the output of a θ-independent channel C with input $\mathbf{X}$. See Figure 1. Mathematically, this means that the conditional density of $\mathbf{Y}$ given $\mathbf{X}$ is *functionally independent* of θ. Observe that this definition of complete data is more general than the standard definition, e.g. as used in [4, 24], since it permits the complete and incomplete data to be related through a stochastic mapping. Our definition of complete data reduces to the standard definition when the channel C is specialized to a *noiseless channel*, i.e. a deterministic many-to-one transformation h such that $\mathbf{Y} = h(\mathbf{X})$.

Let the random variable $\mathbf{X}$ take values $\{\mathbf{x}\}$ in a set $\mathcal{X}$ and let $\mathbf{X}$ have p.d.f. $f(\mathbf{x}; \theta)$. Then for an initial point θ^0 the EM algorithm produces a sequence of points $\{\theta^i\}_{i=1}^{\infty}$ via one of the recursions:

$$\theta^{i+1} = \begin{cases} \text{argmax}_\theta \{Q(\theta, \theta^i)\}, & i = 1, 2, \ldots \\ or & \\ \text{argzero}_\theta \left\{\nabla^{10} Q(\theta, \theta^i)\right\}, & i = 1, 2, \ldots \end{cases} \tag{25}$$

where $Q(\theta, \overline{\theta})$ is the conditional expectation of the complete data log-likelihood function minus the penalty:

$$Q(\theta, \overline{\theta}) \quad \stackrel{\text{def}}{=} \quad E\{\ln f(\mathbf{X}; \theta) | \mathbf{Y} = \mathbf{y}; \overline{\theta}\} - P(\theta). \tag{26}$$

The recursion (25) is a special case of the A algorithm (1) and thus convergence can be investigated using Theorem 1.

Using the elementary identity $f(\mathbf{x}; \theta) = \frac{f(\mathbf{X}|\mathbf{y}; \theta) f(\mathbf{y}; \theta)}{f(\mathbf{y}|\mathbf{X}; \theta)}$ and the property that $f(\mathbf{y}|\mathbf{x}; \theta) = f(\mathbf{y}|\mathbf{x})$ is independent of θ the Q function in the EM algorithm (25) takes the equivalent form:

$$Q(\theta, \overline{\theta}) \quad = \quad \ln f(\mathbf{y}; \theta) + E\{\ln f(\mathbf{X}|\mathbf{y}; \theta) | \mathbf{Y} = \mathbf{y}; \overline{\theta}\}$$

$$
\begin{aligned}
& -E\{\ln f(\mathbf{y}|\mathbf{X})|\mathbf{Y}=\mathbf{y};\overline{\theta}\} - P(\theta) \\
= \;& L(\theta) + H(\theta,\overline{\theta}) - W(\overline{\theta}) - P(\theta).
\end{aligned}
$$

Here $H(\theta,\overline{\theta}) = E\{\ln f(\mathbf{X}|\mathbf{y};\theta)|\mathbf{Y}=\mathbf{y};\overline{\theta}\}$ is the (negative) complete-data conditional entropy and $W(\overline{\theta})$ is a function independent of θ. The above Q function differs from the standard penalized ML-EM Q function of [4, 9] in only one respect: the presence of the function $W(\overline{\theta})$. For the standard case, the mapping from complete to incomplete data is deterministic, $f(\mathbf{y}|\mathbf{X};\theta)$ is degenerate, and $W(\overline{\theta}) = 0$. Since $E\{\ln f(\mathbf{X}|\mathbf{y};\overline{\theta})|\mathbf{Y}=\mathbf{y};\overline{\theta}\}$ and $W(\overline{\theta})$ are functionally independent of θ, an equivalent form for the Q function in the penalized ML-EM algorithm (25) is:

$$
Q(\theta,\overline{\theta}) \;=\; L(\theta) - D(\theta\|\overline{\theta}) - P(\theta) \tag{27}
$$

where $D(\theta\|\overline{\theta})$ is the *Kullback-Liebler (KL) discrimination*:

$$
D(\theta\|\overline{\theta}) \stackrel{\text{def}}{=} \int \ln \frac{f(\mathbf{x}|\mathbf{y};\overline{\theta})}{f(\mathbf{x}|\mathbf{y};\theta)} f(\mathbf{x}|\mathbf{y};\overline{\theta})d\mathbf{x}.. \tag{28}
$$

The following properties of the KL discrimination $D(\theta\|\overline{\theta})$ follow directly from [15, Ch. 2]:

1. $D(\theta\|\overline{\theta}) \geq 0$ where "=" holds iff $g(\mathbf{x}|\mathbf{y};\theta) = g(\mathbf{x}|\mathbf{y};\overline{\theta})$ a.e. in $\mathbf{x}$.
2. When differentiation of $f(\mathbf{x}|\mathbf{y};\theta)$ under the integral sign is justified [15, Sec. 2.6]:
   (a) $\nabla^{10}D(\theta\|\theta) = \nabla^{01}D(\theta\|\theta) = 0$
   (b) $\nabla^{20}D(\theta\|\theta) \geq 0$
   (c) $-\nabla^{11}D(\theta\|\theta) = \nabla^{20}D(\theta\|\theta)$
3. $\nabla^{20}D(\theta\|\theta) = F_{X|\mathbf{y}}(\theta)$, where

   $$F_{X|\mathbf{y}}(\theta) \stackrel{\text{def}}{=} E\{-\nabla^2_\theta \log f(\mathbf{X}|\mathbf{y};\theta)|\mathbf{Y}=\mathbf{y};\theta\}.$$

   is the non-negative definite conditional Fisher information.

The representation (27) immmediately gives:

Lemma 2 *The penalized ML-EM algorithm with stochastic mapping (25) generates a sequence* $\{\theta^i\}_{i=1}^\infty$ *for which the penalized ML estimate* $\hat{\theta} = \mathbf{argmax}_\theta\{L(\theta) - P(\theta)\}$ *is a fixed point. Furthermore, for any initial point* θ^0 *the penalized likelihood is non-decreasing at each step in the sense that:*

$$
L(\theta^{i+1}) - P(\theta^{i+1}) \geq L(\theta^i) - P(\theta^i), \qquad i = 0, 1, \ldots.
$$

Proof of Lemma 2:

Fix i and let $\theta^i = \hat{\theta}$. Then:

$$\theta^{i+1} = \mathop{\mathbf{argmax}}_{\theta}\{L(\theta) - D(\theta\|\hat{\theta}) - P(\theta)\}$$

Since $L(\theta) - P(\theta)$ and $-D(\theta\|\hat{\theta})$ individually take their maximum values at the same point $\theta = \hat{\theta}$ we have $\theta^{i+1} = \theta^i = \hat{\theta}$. By induction we thus obtain $\theta^n = \hat{\theta}$ for all $n > i$. The monotonic increase in penalized likelihood follows from the chain of inequalities:

$$\begin{aligned} 0 &\leq Q(\theta^{i+1}, \theta^i) - Q(\theta^i, \theta^i) \\ &= (L(\theta^{i+1}) - P(\theta^{i+1})) - (L(\theta^i) - P(\theta^i)) \\ &\quad -D(\theta^{i+1}, \theta^i) + D(\theta^i, \theta^i) \\ \\ &\leq (L(\theta^{i+1}) - P(\theta^{i+1})) - (L(\theta^i) - P(\theta^i)) \end{aligned}$$

where the last inequality is a consequence of the inequality: $D(\theta, \theta^i) \geq D(\theta^i, \theta^i) = 0$ for all θ. □

We will need the following definitions:

Definition 2 *For $\hat{\theta} = \mathbf{argmax}_\theta\{L(\theta) - P(\theta)\}$ the penalized ML estimate define the symmetric Hessian matrices:*

$$\begin{aligned} \mathbf{Q} &\stackrel{\text{def}}{=} -\nabla^{20} Q(\hat{\theta}, \hat{\theta}) \\ \mathbf{L} &\stackrel{\text{def}}{=} -\nabla^2_{\hat{\theta}} L(\hat{\theta}) \\ \mathbf{P} &\stackrel{\text{def}}{=} \nabla^2_{\hat{\theta}} P(\hat{\theta}) \\ \mathbf{D} &\stackrel{\text{def}}{=} \nabla^{20} D(\hat{\theta}\|\hat{\theta}). \end{aligned} \tag{29}$$

The following relations follow directly from (27) and properties of the KL discrimination:

$$\begin{aligned} \mathbf{Q} &= \mathbf{L} + \mathbf{P} + \mathbf{D} \\ \nabla^{11} Q(\hat{\theta}, \hat{\theta}) &= -\mathbf{D}. \end{aligned} \tag{30}$$

Theorem 2 *Assume: i) the penalized ML estimate $\hat{\theta} = \mathbf{argmax}_\theta\{L(\theta) - P(\theta)\}$ occurs in the interior of the set Θ; ii) for all $\overline{\theta} \in \Theta$, the maximum $\max_\theta Q(\theta, \overline{\theta})$ is achieved on the interior of the set Θ; iii) $L(\theta)$, $P(\theta)$, and $D(\theta\|\overline{\theta})$ are twice continuously differentiable in $\theta \in \Theta$ and $\overline{\theta} \in \Theta$ and $\mathbf{L} + \mathbf{P} = -\nabla^2_{\hat{\theta}}[L(\hat{\theta}) - P(\hat{\theta})] > 0$. Let the point θ^0 initialize the EM algorithm with stochastic mapping (25).*

1. *If the positivity condition (8) is satisfied then the sucessive differences* $\Delta\theta^i = \theta^i - \hat{\theta}$ *of the A algorithm obey the recursion (10).*

2. *If* $\theta^0 \in \mathcal{R}_+$ *then* $\|\Delta\theta^i\|$ *converges monotonically to zero with at least linear rate and*

3. $\Delta\theta^i$ *asymptotically converges to zero with root convergence factor*

$$\rho\left(\mathbf{I} - \mathbf{Q}^{-1}[\mathbf{L}+\mathbf{P}]\right) = \left\|\mathbf{I} - \mathbf{Q}^{-\frac{1}{2}}[\mathbf{L}+\mathbf{P}]\mathbf{Q}^{-\frac{1}{2}}\right\|_2$$

which is strictly less than one.

Proof of Theorem 2

By Lemma 2, in the notation of Theorem 1, the EM algorithm has a fixed point at $\theta^* = \hat{\theta}$. Furthermore, since $Q(\theta,\overline{\theta}) = L(\theta) - D(\theta\|\overline{\theta}) - P(\theta)$, assumption iii of Theorem 2 guarantees that $Q(\theta,\overline{\theta})$ is twice continuously differentiable in both arguments. Thus the assumptions of Theorem 1 are satisfied and item 1 of Theorem 2 follows. Now by Theorem 1 the root convergence factor is given by $\rho\left(-[\nabla^{20}Q(\hat{\theta},\hat{\theta})]^{-1}\nabla^{11}Q(\hat{\theta},\hat{\theta})\right)$. ¿From identities (29) and (30) $-[\nabla^{20}Q(\hat{\theta},\hat{\theta})]^{-1}\nabla^{11}Q(\hat{\theta},\hat{\theta}) = \mathbf{Q}^{-1}\mathbf{D} = [\mathbf{D}+\mathbf{L}+\mathbf{P}]^{-1}\mathbf{D} = \mathbf{I} - \mathbf{Q}^{-1}[\mathbf{L}+\mathbf{P}]$. Since $\mathbf{L}+\mathbf{P}$ is positive definite and $\mathbf{D}$ is non-negative definite (property 2.b of the KL discrimination), Lemma 3 (Appendix) asserts that the eigenvalues of $\mathbf{Q}^{-1}\mathbf{D}$ are in the range $[0,1)$. Furthermore, $\mathbf{I} - \mathbf{Q}^{-1}[\mathbf{L}+\mathbf{P}]$ is similar to the symmetric matrix $\mathbf{I} - \mathbf{Q}^{-\frac{1}{2}}[\mathbf{L}+\mathbf{P}]\mathbf{Q}^{-\frac{1}{2}}$ and therefore these two matrices have identical eigenvalues. Since $\rho(\mathbf{A}) = \|\mathbf{A}\|_2$ for any real symmetric non-negative matrix $\mathbf{A}$ the theorem follows. $\Box$

Note that when the penalty function induces coupling between parameters, the M-step of the EM "algorithm" described above can be intractable. The OSL method of Green and the majorization method of DePierro, both described below, address this difficulty by modifying the Q function.

III.b: Linear Approximation to ML-EM Algorithm

In [2] the unpenalized ML-EM algorithm was formulated for the difficult case of intensity parameter estimation for continuous-time filtered Poisson-Gaussian observations. By selecting the complete data as the unobservable Poisson increment process $\{d\mathbf{N}_t\}_{t\in[0,T]}$ over the time interval $[0,T]$, an ML-EM algorithm was derived of the form:

$$\theta^{i+1} = \underset{\theta}{\mathbf{argmax}}\, Q(\theta,\theta^i), \qquad i = 1,2,\ldots \tag{31}$$

where

$$Q(\theta,\overline{\theta}) \stackrel{\text{def}}{=} \int_0^T \hat{\lambda}(t|\mathbf{y};\overline{\theta}) \ln \lambda(t|\theta) dt \tag{32}$$

and $\lambda(t|\theta)$ is the Poisson point process intensity over time $t \in [0, T]$ and parameterized by θ, and $\hat{\lambda}(t|\mathbf{y}; \overline{\theta}) = E\{d\mathbf{N}_t|\mathbf{Y} = \mathbf{y}; \overline{\theta}\}$ is the conditional expectation of the Poisson increment process given $\mathbf{Y} = \mathbf{y}$ and $\theta = \overline{\theta}$, i.e. the minimum mean-square error estimate of $\mathbf{N}_t$. Unfortunately the computation of the conditional mean estimator proved to be intractible and instead the best linear estimator $\tilde{\lambda}(t; \theta|\mathbf{y}; \overline{\theta})$ was substituted into (32):

$$\tilde{Q}(\theta, \overline{\theta}) \quad \stackrel{\text{def}}{=} \quad \int_0^T \tilde{\lambda}(t|\mathbf{y}; \overline{\theta}) \ln \lambda(t|\theta) dt$$

While the algorithm resulting from replacing Q by $\tilde{Q}$ is no longer an ML-EM algorithm, and the ML estimate may not even be a fixed point, it belongs to the class of A algorithms (1) for which Theorem 1 can be applied to establish monotone convergence properties and asymptotic convergence rate. In particular, with θ^* a fixed point, the asymptotic convergence rate to θ^* is $\rho\left([\nabla^{20}\tilde{Q}(\theta^*, \theta^*)]^{-1}\nabla^{11}\tilde{Q}(\theta^*, \theta^*)\right)$.

III.c: One-Step-Late (OSL) Penalized ML-EM

Green [9, 10] proposed an approximation, which he called the one-step-late (OSL) algorithm, for the case of tomographic image reconstruction with Poisson data and a Gibbs prior for which the M step of the penalized ML-EM algorithm is intractible. Green's algorithm is equivalent to linearizing the prior $\ln f(\theta)$ about the previous iterate θ^i in (25):

$$\theta^{i+1} = \left\{ \begin{array}{ll} \text{argmax}_\theta \left\{ E\{\ln f(\mathbf{X}; \theta)|\mathbf{Y}; \theta^i\} + \nabla_{\theta^i} \ln f(\theta^i)(\theta - \theta^i) \right\}, & i = 1, 2, \ldots \\ or & \\ \text{argzero}_\theta \left\{ \nabla_\theta E\{\ln f(\mathbf{X}; \theta)|\mathbf{Y}; \theta^i\} + \nabla_{\theta^i} f(\theta^i) \right\}, & i = 1, 2, \ldots \end{array} \right. . \tag{33}$$

Again Theorem 1 is applicable by identifying Q in the theorem with the function $E\{\ln f(\mathbf{X}; \theta)|\mathbf{Y}; \theta^i\} + \nabla_{\theta^i} \ln f(\theta^i)(\theta - \theta^i)$ in (33). If the OSL algorithm converges to a fixed point θ^* the asymptotic convergence rate is:

$$\rho\left([\nabla^{20}Q(\theta^*, \theta^*)]^{-1}[\nabla^{11}Q(\theta^*, \theta^*) + \nabla^2_{\theta^i} \ln f(\theta^*)]\right) \quad = \quad \rho\left([\mathbf{L} + \mathbf{D}]^{-1}[\mathbf{D} - \mathbf{P}]\right)$$

which is identical to the result cited in [10] for the standard case of deterministic complete/incomplete data mapping and the Gibbs prior $f(\theta) = \exp\{-\beta V(\theta)\}$.

IV. APPLICATIONS

We consider two separate applications: the linear Gaussian model and the PET image reconstruction model. These two cases involve complete and incomplete data sets with Gaussian/Gaussian and Poisson/Poisson statistics, respectively.

IV.a. Linear Gaussian Model

Consider the following linear Gaussian model:

$$\mathbf{Y} = \mathbf{G}\theta + \mathbf{W}_y \tag{34}$$

where $\theta \in \Theta = \mathbb{R}^p$ is a p-element parameter vector, $\mathbf{G}$ is an $m \times p$ matrix with full column rank $p \leq m$, and $\mathbf{W}_y$ is an m-dimensional zero mean Gaussian noise with positive definite covariance Λ_{yy}. The unpenalized ML estimator of θ given $\mathbf{Y}$ is the weighted least squares estimator:

$$\hat{\theta} = [\mathbf{G}^T \Lambda_{yy}^{-1} \mathbf{G}]^{-1} \mathbf{G}^T \Lambda_{yy}^{-1} \mathbf{Y}. \tag{35}$$

Next consider decomposing the matrix $\mathbf{G}$ into the matrix product $\mathbf{BC}$ where the $m \times n$ matrix $\mathbf{B}$ has full row rank m, the $n \times p$ matrix $\mathbf{C}$ has full column rank p, and $p \leq m \leq n$. With this decomposition we can define a complete-incomplete data model associated with (34):

$$\begin{aligned} \mathbf{Y} &= \mathbf{BX} + \mathbf{W} && (36) \\ \mathbf{X} &= \mathbf{C}\theta + \mathbf{W}_x && (37) \end{aligned}$$

where the m-element vector $\mathbf{W}$ and the n-element vector $\mathbf{W}_x$ are jointly Gaussian with zero mean and θ-independent positive definite covariance matrix $E_\theta \left\{ \begin{bmatrix} \mathbf{W} \\ \mathbf{W}_x \end{bmatrix} [\mathbf{W} \; \mathbf{W}_x] \right\}$. These assumptions guarantee that θ be identifiable in the noiseless regime when $\mathbf{W}_x$ and $\mathbf{W}$ are vectors of zeroes. The model (36) is of interest to us since the non-zero noise $\mathbf{W}$ case is not covered by the standard ML-EM algorithm assumptions. On the other hand, the Gaussian complete/incomplete data mapping (36) specifies $\mathbf{Y}$ as the output of a simple additive noise channel with input $\mathbf{X}$; a complete-incomplete data model for which our theory directly applies.

For the Gaussian model (36) the conditional distribution of $\mathbf{Y}$ given $\mathbf{X} = \mathbf{x}$ is specified by a m-variate Gaussian density $\mathcal{N}(\mu, \Lambda)$ with vector location parameter:

$$\begin{aligned} \mu &= \mathbf{Bx} + E[\mathbf{W}|\mathbf{X} = \mathbf{x}; \theta] \\ &= \mathbf{Bx} + \Lambda_{yx}\Lambda_{xx}^{-1}[\mathbf{x} - \mathbf{C}\theta] \end{aligned}$$

and matrix scale parameter:

$$\Lambda = \Lambda_{yy} - \Lambda_{xy}^T \Lambda_{xx}^{-1} \Lambda_{xy}.$$

By assumption the scale parameter Λ is functionally independent of θ. However, unless $\Lambda_{nx} = 0$ the location parameter μ generally depends on θ. To ensure that the conditional density of $\mathbf{Y}$ given $\mathbf{X} = \mathbf{x}$ be independent of θ it is required that $\mathbf{W}$ and $\mathbf{W}_x$ be uncorrelated. Under this condition (36) is a valid complete-incomplete data model.

The complete data log-likelihood is:

$$\ln f(\mathbf{x};\theta) = -\tfrac{1}{2}(\mathbf{x}-\mathbf{C}\theta)^T\Lambda_{xx}^{-1}(\mathbf{x}-\mathbf{C}\theta) - \tfrac{1}{2}\ln|\Lambda_{xx}|.$$

Now the unpenalized ML-EM algorithm is of the form (25) with:

$$\begin{aligned}
Q(\theta,\overline{\theta}) &= E[\ln f(\mathbf{X};\theta)|\mathbf{Y};\overline{\theta}] \\
&= -\tfrac{1}{2}(E[\mathbf{X}|\mathbf{Y};\overline{\theta}]-\mathbf{C}\theta)^T\Lambda_{xx}^{-1}(E[\mathbf{X}|\mathbf{Y};\overline{\theta}]-\mathbf{C}\theta) \\
&\quad -\tfrac{1}{2}E\left[(\mathbf{X}-E[\mathbf{X}|\mathbf{Y};\overline{\theta}])^T\Lambda_{xx}^{-1}(\mathbf{X}-E[\mathbf{X}|\mathbf{Y};\overline{\theta}])\,\Big|\mathbf{Y};\overline{\theta}\right] - \tfrac{1}{2}\ln|\Lambda_{xx}| \\
&= -\tfrac{1}{2}(E[\mathbf{X}|\mathbf{Y};\overline{\theta}]-\mathbf{C}\theta)^T\Lambda_{xx}^{-1}(E[\mathbf{X}|\mathbf{Y};\overline{\theta}]-\mathbf{C}\theta) + K(\mathbf{Y};\overline{\theta})
\end{aligned} \tag{38}$$

where $K(\mathbf{Y};\overline{\theta})$ is functionally independent of θ. The conditional expectation in (38) has the form:

$$E[\mathbf{X}|\mathbf{Y};\theta^i] = [\mathbf{I}-\Lambda_{xy}\Lambda_{yy}^{-1}\mathbf{B}]\mathbf{C}\cdot\theta^i + \Lambda_{xy}\Lambda_{yy}^{-1}\mathbf{Y} \tag{39}$$

$$\quad = [\mathbf{I}-\Lambda_{xx}\mathbf{B}^T\Lambda_{yy}^{-1}\mathbf{B}]\mathbf{C}\cdot\theta^i + \Lambda_{xx}\mathbf{B}^T\Lambda_{yy}^{-1}\mathbf{Y}. \tag{40}$$

It is easily verified that:

$$\begin{aligned}
-\nabla^{20}Q(\theta,\overline{\theta}) &= \mathbf{C}^T\Lambda_{xx}^{-1}\mathbf{C} \\
&= \mathbf{F}_X
\end{aligned}$$

and

$$\nabla^{11}Q(\theta,\overline{\theta}) = \mathbf{C}^T\Lambda_{xx}^{-1}\mathbf{C} - \mathbf{C}^T\mathbf{B}^T\Lambda_{yy}^{-1}\mathbf{B}\mathbf{C} \tag{41}$$

$$\quad = \mathbf{C}^T\Lambda_{xx}^{-1}\mathbf{C} - \mathbf{C}^T\mathbf{B}^T[\mathbf{B}\Lambda_{xx}\mathbf{B}^T+\Lambda_{nn}]^{-1}\mathbf{B}\mathbf{C} \tag{42}$$

$$\quad = \mathbf{F}_X - \mathbf{F}_{X|y} \tag{43}$$

where $\mathbf{F}_X = E\{-\nabla_\theta^2 \ln f(\mathbf{X};\theta)\}$ and $\mathbf{F}_{X|y} = E\{-\nabla_\theta^2 \ln f(\mathbf{X}|\mathbf{Y};\theta)|\mathbf{Y}=y;\theta\}$ are unconditional and conditional Fisher information matrices associated with $\mathbf{X}$.

Since the matrices $\nabla^{11}Q$ and $\nabla^{20}Q$ are functionally independent of θ and $\overline{\theta}$ the matrices $A_1 = \mathcal{A}_1 = M_1$ and $A_2 = \mathcal{A}_2 = M_2$ defined in (6) and (7) are given by the θ- and $\overline{\theta}$-independent matrices:

$$M_1(\theta,\overline{\theta}) = \mathbf{F}_X$$
$$M_2(\theta,\overline{\theta}) = \mathbf{F}_X - \mathbf{F}_{X|y}.$$

Now the condition $M_1(\theta,\overline{\theta}) > 0$ (8) is satisfied since $\mathbf{C}$ is full rank. Thus we obtain from Theorem 2 the recursion for $\Delta\theta^i = \theta^i - \hat{\theta}$:

$$\Delta\theta^{i+1} = \mathbf{F}_X^{-1}[\mathbf{F}_X - \mathbf{F}_{X|y}]\cdot\Delta\theta^i$$

This is equivalent to:

$$\mathbf{F}_X^{\frac{1}{2}}\Delta\theta^{i+1} = \mathbf{F}_X^{-\frac{1}{2}}[\mathbf{F}_X - \mathbf{F}_{X|y}]\mathbf{F}_X^{-\frac{1}{2}}\cdot\mathbf{F}_X^{\frac{1}{2}}\Delta\theta^i. \tag{44}$$

Take the Euclidean norm of both sides of (44) to obtain:

$$\|\Delta\theta^{i+1}\| \quad \leq \quad \left\| \mathbf{F}_X^{-\frac{1}{2}}[\mathbf{F}_X - \mathbf{F}_{X|y}]\mathbf{F}_X^{-\frac{1}{2}} \right\|_2 \cdot \|\Delta\theta^i\| \tag{45}$$

where $\|\cdot\|_2$ is the matrix-2 norm and $\|\cdot\|$ is the weighted Euclidean norm defined on vectors $u \in \mathbb{R}^p$:

$$\|u\| \stackrel{\text{def}}{=} u^T \mathbf{F}_X u. \tag{46}$$

Applying the Sherman-Morrisey-Woodbury [7] identity to the matrix $\mathbf{F}_X - \mathbf{F}_{X|y}$ (43) we see that it is symmetric positive definite:

$$\begin{aligned} \Delta\mathbf{F} &\stackrel{\text{def}}{=} \mathbf{F}_X - \mathbf{F}_{X|y} \\ &= \mathbf{C}^T[\Lambda_{xx}^{-1} - \mathbf{B}^T[\mathbf{B}\Lambda_{xx}\mathbf{B} + \Lambda_{nn}]^{-1}\mathbf{B}]\mathbf{C} = \mathbf{C}^T\Lambda_{xx}^{-1}[\Lambda_{xx}^{-1} + \mathbf{B}^T\Lambda_{nn}^{-1}\mathbf{B}]^{-1}\Lambda_{xx}^{-1}\mathbf{C} \\ &> 0. \end{aligned} \tag{47}$$

Thus $\mathbf{F}_X^{-\frac{1}{2}}[\mathbf{F}_X - \mathbf{F}_{X|y}]\mathbf{F}_X^{-\frac{1}{2}}$ is symmetric positive definite and therefore:

$$\begin{aligned} \left\| \mathbf{F}_X^{-\frac{1}{2}}[\mathbf{F}_X - \mathbf{F}_{X|y}]\mathbf{F}_X^{-\frac{1}{2}} \right\|_2 &= \rho\left(\mathbf{F}_X^{-\frac{1}{2}}[\mathbf{F}_X - \mathbf{F}_{X|y}]\mathbf{F}_X^{-\frac{1}{2}}\right) \\ &= \rho\left(\mathbf{I} - \mathbf{F}_X^{-1}\mathbf{F}_{X|y}\right) \\ &= \rho\left(\mathbf{I} - [\Delta\mathbf{F} + \mathbf{F}_{X|y}]^{-1}\mathbf{F}_{X|y}\right) \\ &< 1 \end{aligned}$$

where we have used Lemma 3 and the fact that $\Delta\mathbf{F} > 0$ and $\mathbf{F}_{X|y} \geq 0$. Therefore from (45):

$$\|\Delta\theta^{i+1}\| < \|\Delta\theta^i\|$$

and the ML-EM algorithm converges monotonically in the norm $\|\cdot\|$ (46) for all initial points θ^0. Therefore it converges globally in any norm. The asymptotic convergence rate is seen to be $\rho\left(\mathbf{I} - \mathbf{F}_X^{-1}\mathbf{F}_{X|y}\right)$. We have thus established the following:

Theorem 3 *The ML-EM algorithm for the Gaussian complete/incomplete data mapping defined by (36) globally converges everywhere in $\Theta = \mathbb{R}^p$ to the ML estimate. Furthermore convergence is monotone in the norm $\|u\| \stackrel{\text{def}}{=} u^T\mathbf{F}_X u$ and the root convergence factor is $\rho(\mathbf{A}) < 1$ where $\mathbf{A}$ is the matrix:*

$$\mathbf{A} \quad = \quad \mathbf{I} - \mathbf{F}_X^{-1}\mathbf{F}_{X|y} \tag{48}$$

where

$$\mathbf{F}_X \quad \stackrel{\text{def}}{=} \quad \mathbf{C}^T\Lambda_{xx}^{-1}\mathbf{C} \tag{49}$$

$$\mathbf{F}_{X|y} \quad \stackrel{\text{def}}{=} \quad \mathbf{C}^T\mathbf{B}^T[\mathbf{B}\Lambda_{xx}\mathbf{B} + \Lambda_{nn}]^{-1}\mathbf{B}\mathbf{C}. \tag{50}$$

Finally, it is useful to remark that due to the form of $\mathbf{A}$ (48), the spectral radius $\rho(\mathbf{A})$ can only increase as the covariance Λ_{nn} of the channel noise $\mathbf{W}$ increases. We therefore conclude that while increased channel noise does not affect the region of monotone convergence of the ML-EM algorithm it does adversely affect the rate of convergence for the Gaussian model (36).

IV.b. PET Image Reconstruction

In the PET problem the objective is to estimate the intensity $\theta = [\theta_1, \ldots, \theta_p]^T$, $\theta_b \geq 0$, governing the number of gamma-ray emissions $\mathbf{N} = [\mathbf{N}_1, \ldots, \mathbf{N}_p]^T$ over an imaging volume of p pixels. The estimate of θ must be based on the projection data $\mathbf{Y} = [\mathbf{Y}_1, \ldots, \mathbf{Y}_m]^T$. Both $\mathbf{N}$ and $\mathbf{Y}$ are Poisson distributed:

$$P(\mathbf{N}; \theta) = \prod_{b=1}^{p} \frac{[\theta_b]}{\mathbf{N}_b!}^{\mathbf{N}_b} e^{-\theta_b},$$

$$P(\mathbf{Y}; \theta) = \prod_{d=1}^{m} \frac{[\mu_d]}{\mathbf{Y}_d!}^{\mathbf{Y}_d} e^{-\mu_d} \tag{51}$$

where $\mu_d = E_\theta[\mathbf{Y}_d]$ is the Poisson intensity for detector d:

$$\mu_d = \sum_{b=1}^{p} P_{d|b}\theta_b$$

and $P_{d|b}$ is the transition probability corresponding to emitter location b and detector location d. To ensure a unique ML estimate we assume that $m \geq p$, the $m \times p$ system matrix $[[P_{d|b}]]$ is full rank, and $(\mu_d, \mathbf{Y}_d)$ are strictly positive for all $d = 1, \ldots, m$.

The standard choice of complete data $\mathbf{X}$ for estimation of θ via the EM algorithm is the set $\{\mathbf{N}_{db}\}_{d=1,b=1}^{m,p}$, where $\mathbf{N}_{db}$ denotes the number of emissions in pixel b which are detected at detector d [23, 17]. This complete data is related to the incomplete data via the deterministic many-to-one mapping: $\mathbf{N}_d = \sum_{b=1}^{p} \mathbf{N}_{db}$, $d = 1, \ldots, m$. It is easily established that $\{\mathbf{N}_{db}\}$ are independent Poisson random variables with intensity $E_\theta\{\mathbf{N}_{db}\} = P_{d|b}\theta_b$, $d = 1, \ldots, m$, $b = 1, \ldots, p$ and that the conditional expectation $E\{\ln f(\mathbf{X}; \theta)|\mathbf{y}; \theta^i\}$ of the complete data log-likelihood given the incomplete data is [10]:

$$E\{\ln f(\mathbf{X}; \theta)|\mathbf{Y}; \theta^i\} = \sum_{d=1}^{m}\sum_{b=1}^{p}\left[\frac{\mathbf{Y}_d P_{d|b}\theta_b^i}{\mu_d^i}\ln(P_{d|b}\theta_b) - P_{d|b}\theta_b\right]$$

where $\mu_d^i = \sum_{b=1}^{p} \theta_b^i P_{b|d}$. For a penalty function $P(\theta)$ the Q function for the penalized ML-EM algorithm is:

$$Q(\theta, \theta^i) = E\{\ln f(\mathbf{X}; \theta)|\mathbf{Y}; \theta^i\} - P(\theta),$$

which yields a sequence of estimates θ^i, $i = 1, 2, \ldots$ of θ. In order to obtain asymptotic convergence properties using Theorem 2 it will be necessary to assume θ^i lies on the interior of Θ, i.e. θ^i lies in the strictly positive orthant, for all $i > 0$. This assumption only holds when the unpenalized or penalized ML estimate $\hat{\theta}$ lies in the interior of Θ, a condition which is usually not met throughout the image. For example, when $\sum_{d=1}^m P_{b|d} = 0$ the pixel b is outside the field of view and it is easily established that $\hat{\theta}_b = 0$. Therefore, for the following analysis to hold, the pixels for which $\hat{\theta}$ lies on the boundary must be eliminated from the vector θ^i.

Under these assumptions

$$\begin{aligned} -\nabla^{20} Q(\theta, \theta^i) &= \operatorname{diag}_b\left(\frac{\theta_b^i}{\theta_b}\right) \cdot [\mathbf{B}(\theta^i) + \mathbf{C}(\theta^i)] \cdot \operatorname{diag}_b\left(\frac{\theta_b^i}{\theta_b}\right) + \mathbf{P}(\theta) && (52) \\ \nabla^{11} Q(\theta, \theta^i) &= \operatorname{diag}_b\left(\frac{\theta_b^i}{\theta_b}\right) \cdot \mathbf{C}(\theta^i) && (53) \end{aligned}$$

where, similar to the definition in [10], $\mathbf{B}(\theta^i)$ is the positive definite $p \times p$ matrix:

$$\mathbf{B}(\theta^i) \stackrel{\text{def}}{=} \sum_{d=1}^m \frac{\mathbf{Y}_d}{[\mu_d^i]^2} \underline{P}_{d|*} \underline{P}_{d|*}^T,$$

$\mathbf{B}(\theta^i) + \mathbf{C}(\theta^i)$ is the $p \times p$ positive definite matrix

$$\mathbf{B}(\theta^i) + \mathbf{C}(\theta^i) \stackrel{\text{def}}{=} \operatorname{diag}_b\left(\frac{1}{\theta_b^i} \sum_{d=1}^m \frac{\mathbf{Y}_d P_{d|b}}{\mu_d^i}\right).$$

and

$$\mathbf{P}(\theta) \stackrel{\text{def}}{=} \nabla_\theta^2 P(\theta).$$

The matrices $\mathcal{A}_1(\theta, \theta^i)$ and $\mathcal{A}_2(\theta, \theta^i)$ defined in (7) are obtained by taking the k-th row of $-\nabla^{20} Q(\theta, \theta^i)$ and the k-th row of $\nabla^{11} Q(\theta, \theta^i)$ and replacing θ and θ^i with $\theta(t) = t_k\theta + (1 - t_k)\hat{\theta}$ and $\theta^i(t) = t_k\theta^i + (1 - t_k)\hat{\theta}$, respectively, $k = 1, \ldots, p$. This gives:

$$\begin{aligned} \mathcal{A}_1(\theta, \theta^i) &= \operatorname{diag}_b\left(\frac{\theta_b^i(t_b)}{\theta_b(t_b)}\right) \cdot [\mathbf{B}_t + \mathbf{C}_t] \cdot \operatorname{diag}_b\left(\frac{\theta_b^i(t_b)}{\theta_b(t_b)}\right) + \mathbf{P}_t && (54) \\ \mathcal{A}_2(\theta, \theta^i) &= \operatorname{diag}_b\left(\frac{\theta_b^i(t_b)}{\theta_b(t_b)}\right) \cdot \mathbf{C}_t && (55) \end{aligned}$$

where $\mathbf{P}_t$ is the $p \times p$ matrix:

$$\mathbf{P}_t \stackrel{\text{def}}{=} -\begin{bmatrix} \nabla_\theta \frac{\partial}{\partial\theta_1(t_1)} P(\theta(t_1)) \\ \vdots \\ \nabla_\theta \frac{\partial}{\partial\theta_p(t_p)} P(\theta(t_p)) \end{bmatrix}, \qquad (56)$$

$\mathbf{B}_t$ is the non-negative definite $p \times p$ matrix:

$$\mathbf{B}_t \stackrel{\text{def}}{=} \sum_{d=1}^{m} \mathbf{Y}_d \text{diag}_b \left(\frac{1}{\mu_d^i(t_b)} \right) \underline{P}_{d|*} \underline{P}_{d|*}^T \text{diag}_b \left(\frac{1}{\mu_d^i(t_b)} \right), \tag{57}$$

$\mathbf{B}_t + \mathbf{C}_t$ is the positive definite $p \times p$ matrix:

$$\mathbf{B}_t + \mathbf{C}_t \stackrel{\text{def}}{=} \text{diag}_b \left(\frac{1}{\theta_b^i(t_b)} \sum_{d=1}^{m} \frac{\mathbf{Y}_d P_{d|b}}{\mu_d^i(t_b)} \right), \tag{58}$$

and $\mu_d^i(t_b)| \stackrel{\text{def}}{=} \sum_{k=1}^p \theta_k^i(t_b) P_{k|d}$.

Now if $\mathcal{A}_1(\theta, \theta^i)$ is invertible for all θ, and θ^i we have from (10) of Theorem 1:

$$\begin{aligned} \Delta\theta^{i+1} &= -[\mathcal{A}_1(\theta^{i+1}, \theta^i)]^{-1} \mathcal{A}_2(\theta^{i+1}, \theta^i) \cdot \Delta\theta^i \\ &= \text{diag}_b \left(\frac{\theta_b^{i+1}(t_b)}{\theta_b^i(t_b)} \right) \cdot [\mathbf{B}_t + \mathbf{C}_t + \text{diag}_b \left(\frac{\theta_b^{i+1}(t_b)}{\theta_b^i(t_b)} \right) \mathbf{P}_t \text{diag}_b \left(\frac{\theta_b^{i+1}(t_b)}{\theta_b^i(t_b)} \right)]^{-1} \mathbf{C}_t \cdot \Delta\theta^i \end{aligned} \tag{59}$$

where $t = [t_1, \ldots, t_p]^T$ is a function of $\theta^i, \theta^{i+1}, \hat{\theta}$. Unfortunately, it can be shown that for any θ^i, $\sup_{\theta \in \Theta} \| \mathcal{A}_1(\theta, \theta^i)]^{-1} \mathcal{A}_2(\theta, \theta^i) \|$ is unbounded for any Euclidean-type norm of the form $\|u\|^2 = u^T \mathbf{D} u$ where $\mathbf{D}$ is positive definite. Thus the monotone convergence part of Theorem 2 fails to apply. This suggests that to establish monotone convergence properties of the PET EM algorithm, we should consider other parameterizations of θ.

Consider the alternative parameterization defined by the logarithmic transformation g::

$$\tau \quad = \quad \ln \theta = [\ln \theta_1, \ldots, \ln \theta_p]^T.$$

The inverse of the transformation $g(\theta) = \ln \theta$ is the exponential transformation

$$g^{-1}(\tau) \quad = \quad e^{\tau} = [e^{\tau_1}, \ldots, e^{\tau_p}]^T,$$

and the Jacobian is the diagonal matrix with diagonal elements:

$$[J(\tau)]_{bb} = e^{-\tau_b}.$$

Using (54) and (55) we obtain from (22):

$$\begin{aligned} \Delta\tau^{i+1} \quad = \quad & \text{diag}_b \left(e^{-\tau_b^i(t_b)} \right) \left[\tilde{\mathbf{B}}_t + \tilde{\mathbf{C}}_t + \text{diag}_b \left(e^{\tau_b^{i+1}(t_b) - \tau_b^i(t_b)} \right) \tilde{\mathbf{P}}_t \text{diag}_b \left(e^{\tau_b^{i+1}(t_b) - \tau_b^i(t_b)} \right) \right]^{-1} \\ & \cdot \tilde{\mathbf{C}}_t \; \text{diag}_b \left(e^{\tau_b^i(t_b)} \right) \cdot \Delta\tau^i \end{aligned}$$

where $\tilde{\mathbf{B}}_t$, $\tilde{\mathbf{C}}_t$ and $\tilde{\mathbf{P}}_t$ are $\mathbf{B}_t$, $\mathbf{C}_t$ and $\mathbf{P}_t$ of (56)-(58) parameterized in terms of $\tau = \tau(\theta)$ and $\tau(t_b) = t_b \tau + (1 - t_b)\hat{\tau}$, $b = 1, \ldots, p$. Using the facts that $\tau_b = \ln \theta_b$ and $\tau(t_b) = \ln \theta(\bar{t}_b)$ for some $\bar{t}_b \in [0, 1]$, $b = 1, \ldots, p$, we can express the above in terms of the original parameterization to obtain:

$$\Delta \ln \theta^{i+1} \quad = \quad \mathbf{D}_t^{-1} \left[\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^T \mathbf{P}_t \mathbf{R}_t \right]^{-1} \mathbf{C}_t \; \mathbf{D}_t \cdot \Delta \ln \theta^i, \tag{60}$$

where

$$\mathbf{D}_t \stackrel{\rm def}{=} \mathrm{diag}_b \left(\theta_b^i(t_b)\right)$$
$$\mathbf{R}_t \stackrel{\rm def}{=} \mathrm{diag}_b \left(\frac{\theta_b^{i+1}(t_b)}{\theta_b^i(t_b)}\right)$$

and $\Delta \ln \theta$ is the vector:

$$\Delta \ln \theta \stackrel{\rm def}{=} \ln \theta - \ln \hat{\theta}.$$

In (60) we have dropped the overline in $\overline{t}$ for notational simplicity. We divide subsequent treatment into the unpenalized and penalized cases:

Unpenalized ML-EM

For the unpenalized case $\mathbf{P}_t = 0$, so that $\mathbf{B}_t + \mathbf{C}_t + \mathbf{P}_t = \mathbf{B}_t + \mathbf{C}_t$ is symmetric positive definite and we have from (60):

$$\begin{aligned} & [\mathbf{B}_t + \mathbf{C}_t]^{\frac{1}{2}} \mathbf{D}_t \cdot \Delta \ln \theta^{i+1} \\ & \quad = [\mathbf{B}_t + \mathbf{C}_t]^{-\frac{1}{2}} \mathbf{C}_t [\mathbf{B}_t + \mathbf{C}_t]^{-\frac{1}{2}} \cdot [\mathbf{B}_t + \mathbf{C}_t]^{\frac{1}{2}} \mathbf{D}_t \cdot \Delta \ln \theta^i \end{aligned} \tag{61}$$

Taking the Euclidean norm of both sides of (61) we obtain:

$$\begin{aligned} & \left[\Delta \ln \theta^{i+1}\right]^T \ \mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t] \mathbf{D}_t \ \left[\Delta \ln \theta^{i+1}\right] \\ & \quad \leq \left\| [\mathbf{B}_t + \mathbf{C}_t]^{-\frac{1}{2}} \mathbf{C}_t [\mathbf{B}_t + \mathbf{C}_t]^{-\frac{1}{2}} \right\|_2 \\ & \qquad \cdot \left[\Delta \ln \theta^i\right]^T \ \mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t] \mathbf{D}_t \ \left[\Delta \ln \theta^i\right] \\ & \quad = \rho\left([\mathbf{B}_t + \mathbf{C}_t]^{-1} \mathbf{C}_t\right) \cdot \left[\Delta \ln \theta^i\right]^T \ \mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t] \mathbf{D}_t \ \left[\Delta \ln \theta^i\right] \end{aligned} \tag{62}$$

It is easily seen that $\mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t] \mathbf{D}_t$ is the diagonal matrix:

$$\mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t] \mathbf{D}_t \quad = \quad \mathrm{diag}_b \left(\theta_b^i(t_b) \ \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\mu_d^i(t_b)}\right). \tag{63}$$

This establishes:

$$\sum_{b=1}^p \theta_b^i(t_b) \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\mu_d^i(t_b)} \ \left(\ln \frac{\theta_b^{i+1}}{\hat{\theta}_b}\right)^2 \quad \leq \quad \rho\left([\mathbf{B}_t + \mathbf{C}_t]^{-1} \mathbf{C}_t\right) \ \sum_{b=1}^p \theta_b^i(t_b) \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\mu_d^i(t_b)} \ \left(\ln \frac{\theta_b^i}{\hat{\theta}_b}\right)^2.$$

We next consider the asymptotic form of (62) for small $\|\Delta\theta^i\|_2$. By using $\theta_b^i(t_b) = \hat{\theta}_b + t_b \Delta\theta_b^i$ and $\mu_d^i(t_b) = \hat{\mu}_d + O(\|\Delta\theta^i)\|_2)$ we obtain:

$$\begin{aligned}
\mathbf{D}_t^T[\mathbf{B}_t + \mathbf{C}_t]\mathbf{D}_t &= \mathbf{D}^T[\mathbf{B}+\mathbf{C}]\mathbf{D} + O(\|\Delta\theta^i\|_2) \\
&= \mathrm{diag}_b\left(\hat{\theta}_b \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d}\right) + \mathbf{I}\cdot O(\|\Delta\theta^i\|_2), \qquad (64)\\
\rho\left([\mathbf{B}_t + \mathbf{C}_t]^{-1}\mathbf{C}_t\right) &= \rho\left([\mathbf{B}+\mathbf{C}]^{-1}\mathbf{C}\right) + O(\|\Delta\theta^i\|_2) \qquad (65)
\end{aligned}$$

where $\hat{\mu}_d = \sum_{b=1}^p P_{d|b}\hat{\theta}_b$ and $\mathbf{D} = \mathbf{D}_t|_{t=0}$, $\mathbf{C} = \mathbf{C}_t|_{t=0} = \mathbf{C}(\hat{\theta})$, $\mathbf{B} = \mathbf{B}_t|_{t=0} = \mathbf{B}(\hat{\theta})$. It is proven in Appendix B that $\alpha_1^2 \stackrel{\mathrm{def}}{=} \rho([\mathbf{B}+\mathbf{C}]^{-1}\mathbf{C}) < 1$. Using the asymptotic forms (64) and (64) in (62):

$$\begin{aligned}
&\left[\Delta \ln \theta^{i+1}\right]^T \ \mathrm{diag}_b\left(\hat{\theta}_b \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d}\right) \cdot \left[\Delta \ln \theta^{i+1}\right] \ \left[1 + O(\|\Delta\theta^i\|_2)\right] \qquad (66)\\
&\leq \alpha_1^2 \cdot \left[\Delta \ln \theta^i\right]^T \ \mathrm{diag}_b\left(\hat{\theta}_b \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d}\right) \ \left[\Delta \ln \theta^i\right] \cdot \left[1 + O(\|\Delta\theta^i\|_2)\right].
\end{aligned}$$

Identifying the norm $\|\cdot\|$ defined by:

$$\begin{aligned}
\|u\| &\stackrel{\mathrm{def}}{=} u^T \ \mathrm{diag}\left(\hat{\theta}_b \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d}\right) u \\
&= \sum_{b=1}^p \hat{\theta}_b \sum_{d=1}^m \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} \ u_b^2. \qquad (67)
\end{aligned}$$

we have the equivalent form:

$$\left\|\Delta \ln \theta^{i+1}\right\| \cdot \left[1 + O(\|\Delta\theta^i\|_2)\right]. \quad \leq \quad \alpha_1^2 \left\|\Delta \ln \theta^i\right\| \cdot \left[1 + O(\|\Delta\theta^i\|_2)\right]. \qquad (68)$$

Thus if θ^i is sufficently close to $\hat{\theta}$:

$$\left\|\Delta \ln \theta^{i+1}\right\| \quad < \quad \left\|\Delta \ln \theta^i\right\| \qquad (69)$$

Now it is known that the ML-EM PET algorithm converges [9] so that $\|\theta^i - \hat{\theta}\| \to 0$. As long as $\hat{\theta}$ is strictly positive, the relation (68) asserts that in the final iterations of the algorithm the logarithmic differences $\ln\theta^i - \ln\hat{\theta}$ converge monotonically to zero relative to the norm (67). Furthermore the speed of this asymptotic monotone convergence is inversely proportional to $\alpha_1^2 = \rho([\mathbf{B}+\mathbf{C}]^{-1}\mathbf{C})$.

The norm $\|\cdot\|$ in (67) has a simpler equivalent form which is functionally dependent on $\mathbf{Y}_d$ only through $\hat{\theta}$. The PET log-likelihood function $\ln P(\mathbf{Y};\theta)$ (51) has derivative at the maximum likelihood estimate $\hat{\theta}$:

$$\frac{\partial}{\partial\hat{\theta}_b} \ln P(\mathbf{Y};\hat{\theta}) = \sum_{d=1}^p \left(\mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} - P_{d|b}\right), \qquad b = 1,\ldots,p. \qquad (70)$$

Now since $\hat{\theta}$ is a stationary point of $\ln P(\mathbf{Y};\theta)$ this derivative is zero and:

$$\sum_{d=1}^{p} \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} = P_d$$

where

$$P_b \stackrel{\text{def}}{=} \sum_{b=1}^{p} P_{d|b}$$

Thus (69)is equivalent to:

$$\sum_{b=1}^{p} P_b \hat{\theta}_b \left(\ln \theta_b^{i+1} - \ln \hat{\theta}_b\right)^2 \quad < \quad \sum_{b=1}^{p} P_b \hat{\theta}_b \left(\ln \theta_b^{i} - \ln \hat{\theta}_b\right)^2$$

Finally we note that:

$$\Delta \ln \theta = \ln \frac{\theta_b}{\hat{\theta}_b} \quad = \quad \frac{\theta_b - \hat{\theta}_b}{\hat{\theta}_b} + O(|\Delta\theta_b|)$$

so that to $O(\|\Delta\theta^i\|_2)$ (68) is equivalent to:

$$\sum_{b=1}^{p} P_b \left(\frac{\theta_b^{i+1} - \hat{\theta}_b}{\hat{\theta}_b}\right)^2 \; < \; \sum_{b=1}^{p} P_b \left(\frac{\theta_b^{i} - \hat{\theta}_b}{\hat{\theta}_b}\right)^2$$

Assuming the simple case where $P_b = \sum_{d=1}^{m} P_{d|b} = 1$ we conclude that asymptotically the vector of ratios $\Delta\theta^i/\hat{\theta} \stackrel{\text{def}}{=} [\Delta\theta_b^i/\hat{\theta}_b, \ldots, \Delta\theta_b^i/\hat{\theta}_b]^T$ converges monotonically to zero in the standard Euclidean norm.

We summarize these results in the following theorem.

Theorem 4 *Assume that the unpenalized PET ML-EM algorithm converges to the strictly positive limit $\hat{\theta}$. Then, in the final iterations the logarithm of sucessive iterates converge monotonically to $\log \hat{\theta}$ in the sense that for some sufficiently large positive integer M:*

$$\|\log \theta^{i+1} - \log \hat{\theta}\| \leq \alpha_1^2 \|\log \theta^i - \log \hat{\theta}\|, \qquad i \geq M,$$

where $\alpha_1^2 = \rho([\mathbf{B}+\mathbf{C}]^{-1}\mathbf{C})$, $\mathbf{B} = \mathbf{B}(\hat{\theta})$, $\mathbf{C} = \mathbf{C}(\hat{\theta})$, the norm $\|\bullet\|$ is defined as:

$$\|u\| \stackrel{\text{def}}{=} \sum_{b=1}^{p} P_b \hat{\theta}_b \; u_b^2.$$

and $P_b \stackrel{\text{def}}{=} \sum_{d=1}^{m} P_{d|b}$.

Quadratically Penalized ML-EM

We assume that $P(\theta) = \frac{1}{2}\theta^T \Lambda \theta$ where Λ is a symmetric non-negative definite $p \times p$ matrix. There is no known closed form solution to the M-step of the penalized ML-EM algorithm (23) unless Λ is diagonal. Therefore, for non-diagonal Λ the recursion (23) is only a theoretical algorithm. Nonetheless, the convergence properties of this theoretical penalized ML-EM algorithm can be studied using Theorem 2.

Since $\mathbf{B}_t + \mathbf{C}_t$ is positive definite, $\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^T \mathbf{P}_t \mathbf{R}_t = \mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t \Lambda \mathbf{R}_t$ is positive definite and from (60) we have the representation:

$$\begin{aligned}
&[\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^T \Lambda \mathbf{R}_t]^{\frac{1}{2}} \mathbf{D}_t \Delta \ln \theta^{i+1} \\
&\quad = [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{-\frac{1}{2}} \mathbf{C}_t \cdot [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{-\frac{1}{2}} \\
&\qquad \cdot [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{\frac{1}{2}} \mathbf{D}_t \Delta \ln \theta^{i}.
\end{aligned} \tag{71}$$

Taking the Euclidean norm of both sides

$$\begin{aligned}
&[\Delta \ln \theta^{i+1}]^T \; \mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}] \mathbf{D}_t \; [\Delta \ln \theta^{i+1}] \\
&\leq \left\| [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{-\frac{1}{2}} \mathbf{C}_t [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{-\frac{1}{2}} \right\|_2 \\
&\qquad \cdot [\Delta \ln \theta^{i}]^T \; \mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}] \mathbf{D}_t \; [\Delta \ln \theta^{i}] \\
&= \rho \left([\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{-1} \mathbf{C}_t \right) \\
&\qquad \cdot [\Delta \ln \theta^{i}]^T \; \mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}] \mathbf{D}_t \; [\Delta \ln \theta^{i}] .
\end{aligned} \tag{72}$$

As in our study of unpenalized ML-EM we turn to the asymptotic behavior of the penalized ML-EM inequality (72). First observe that as before $\mathbf{D}_t^T [\mathbf{B}_t + \mathbf{C}_t] \mathbf{D}_t = \text{diag}_b \left(\hat{\theta}_b \sum_{d=1} \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} \right) + O(\|\Delta \theta^i\|_2)$ and:

$$\rho \left([\mathbf{B}_t + \mathbf{C}_t + \mathbf{R}_t^{-T} \Lambda \mathbf{R}_t^{-1}]^{-1} \mathbf{C}_t \right) = \rho \left([\mathbf{B} + \mathbf{C} + \Lambda]^{-1} \mathbf{C} \right) + O(\|\Delta \theta^i\|_2).$$

Now it is easily shown that since Λ is non-negative definite: $\alpha_2^2 \stackrel{\text{def}}{=} \rho \left([\mathbf{B} + \mathbf{C} + \Lambda]^{-1} \mathbf{C} \right) \leq \rho \left([\mathbf{B} + \mathbf{C}]^{-1} \mathbf{C} \right) = \alpha_1^2 < 1$. Therefore, similarly to the unpenalized case we have from (72):

$$\begin{aligned}
&[\Delta \ln \theta^{i+1}]^T \left[\text{diag}_b \left(\hat{\theta}_b \sum_{d=1}^{m} \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} \right) + \mathbf{D}^T \Lambda \mathbf{D} \right] [\Delta \ln \theta^{i+1}] \cdot [1 + O(\|\Delta \theta^i\|_2)] \\
&\quad \leq \alpha_2^2 \cdot [\Delta \ln \theta^{i}]^T \left[\text{diag}_b \left(\hat{\theta}_b \sum_{d=1}^{m} \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} \right) + \mathbf{D}^T \Lambda \mathbf{D} \right] [\Delta \ln \theta^{i}] \cdot [1 + O(\|\Delta \theta^i\|_2)] ,
\end{aligned}$$

where $\mathbf{D} \stackrel{\text{def}}{=} \text{diag}_b(\hat{\theta}_b)$. Identifying the norm $\|\cdot\|$ defined by:

$$\|u\| \quad \stackrel{\text{def}}{=} \quad u^T \left[\text{diag} \left(\hat{\theta}_b \sum_{d=1}^{m} \mathbf{Y}_d \frac{P_{d|b}}{\hat{\mu}_d} \right) + \text{diag}_b(\hat{\theta}_b) \Lambda \text{diag}_b(\hat{\theta}_b) \right] u \tag{73}$$

we have:

$$\|\Delta \ln \theta^{i+1}\| \ \cdot \ [1 + O(\|\Delta\theta^i\|_2)] \quad \leq \quad \alpha_1^2 \, \|\Delta \ln \theta^i\| \ \cdot \ [1 + O(\|\Delta\theta^i\|_2)] \, . \tag{74}$$

¿From these results we obtain:

Theorem 5 *Assume that the quadratically penalized PET ML-EM algorithm converges to the strictly positive limit $\hat{\theta}$. Then, in the final iterations the logarithm of sucessive iterates converge monotonically to $\log \hat{\theta}$ in the sense that for some sufficiently large positive integer M:*

$$\|\log \theta^{i+1} - \log \hat{\theta}\| \leq \alpha_2^2 \|\log \theta^i - \log \hat{\theta}\|, \qquad i \geq M,$$

where $\alpha_2^2 \stackrel{\text{def}}{=} \rho\left([\mathbf{B} + \mathbf{C} + \Lambda]^{-1}\mathbf{C}\right) \leq \alpha_1^2 = \rho\left([\mathbf{B} + \mathbf{C}]^{-1}\mathbf{C}\right)$, $\mathbf{B} = \mathbf{B}(\hat{\theta})$, $\mathbf{C} = \mathbf{C}(\hat{\theta})$, and the norm $\|\bullet\|$ is defined by (73).

V. CONCLUSION

We have presented a methodology for studying the asymptotic convergence properties of EM-type algorithms. We have indicated how our methods apply to several important EM and approximate EM algorithms presented in the literature. We have established asymptotic monotone convergence of the log images and asymptotic rate of convergence for the PET ML-EM and penalized ML-EM image reconstruction algorithms. A weakness of the theory given here is that it does not apply to cases where the maximization in the M step is achieved on a boundary of the parameter space. While there are a certain number of such problems where this theory will not apply, we believe that the theory will nonetheless be useful for a large number of applications areas. The theory presented in this paper has recently been applied to evaluating the convergence properties of a rapidly convergent class of EM-type algorithms called space-alternating generalized EM (SAGE) algorithms [6].

APPENDICES

A. Matrix Lemmas

The following matrix results are used in the paper.

Lemma 3 *Let the $p \times p$ symmetric matrices $\mathbf{A}$ and $\mathbf{B}$ be positive definite and non-negative definite, respectively, and define the matrix $\mathbf{C} = \mathbf{A} + \mathbf{B}$. Then the eigenvalues of the matrix $\mathbf{C}^{-1}\mathbf{B}$ all lie in the interval $[0, 1)$.*

Proof: Since the matrix $\mathbf{C}$ is positive definite there exists a symmetric positive definite square root factor $\mathbf{C}^{\frac{1}{2}}$ such that $\mathbf{C} = \mathbf{C}^{\frac{1}{2}}\mathbf{C}^{\frac{1}{2}}$. Furthermore, since $\mathbf{C}^{-\frac{1}{2}}\mathbf{B}\mathbf{C}^{-\frac{1}{2}}$ is non-negative definite: $\mathbf{C}^{-\frac{1}{2}}\mathbf{B}\mathbf{C}^{-\frac{1}{2}} = [\mathbf{I} - \mathbf{C}^{-\frac{1}{2}}\mathbf{A}\mathbf{C}^{-\frac{1}{2}}] \geq 0$. Now adding the fact that $\mathbf{C}^{-\frac{1}{2}}\mathbf{A}\mathbf{C}^{-\frac{1}{2}}$ is positive definite, we obtain $0 \leq \mathbf{C}^{-\frac{1}{2}}\mathbf{B}\mathbf{C}^{-\frac{1}{2}} < \mathbf{I}$ so that all of the eigenvalues of $\mathbf{C}^{-\frac{1}{2}}\mathbf{B}\mathbf{C}^{-\frac{1}{2}}$ are non-negative and strictly less than one. Defining $S = \mathbf{C}^{\frac{1}{2}}$, observe that $\mathbf{C}^{-1}\mathbf{B} = S^{-1} \cdot \mathbf{C}^{-\frac{1}{2}}\mathbf{B}\mathbf{C}^{-\frac{1}{2}} \cdot S$, so that $\mathbf{C}^{-1}\mathbf{B}$ and $\mathbf{C}^{-\frac{1}{2}}\mathbf{B}\mathbf{C}^{-\frac{1}{2}}$ are similar matrices. Since similar matrices have identical eigenvalues $\mathbf{C}^{-1}\mathbf{B}$ has eigenvalues in $[0, 1)$. $\square$

Lemma 4 *Let $\mathbf{B}$ be an $n \times p$ matrix with full column rank $p \leq n$. Then $\rho(\mathbf{A}) < 1$ implies $\rho\left([\mathbf{B}^T\mathbf{B}]^{-1}\mathbf{B}^T\mathbf{A}\mathbf{B}\right) < 1$.*

Proof: We use the following fact: if $\rho(\mathbf{A}) < 1$ then $0 \leq \mathbf{A}\mathbf{A}^T < \mathbf{I}$. The following sequence of inequalities establishes the lemma.

$$
\begin{aligned}
\rho^2\left([\mathbf{B}^T\mathbf{B}]^{-1}\mathbf{B}^T\mathbf{A}\mathbf{B}\right) &= \rho^2\left([\mathbf{B}^T\mathbf{B}]^{-\frac{1}{2}}\mathbf{B}^T\mathbf{A}\mathbf{B}[\mathbf{B}^T\mathbf{B}]^{-\frac{1}{2}}\right) \\
&= \rho\left([\mathbf{B}^T\mathbf{B}]^{-\frac{1}{2}}\mathbf{B}^T\mathbf{A} \cdot \mathbf{B}[\mathbf{B}^T\mathbf{B}]^{-1}\mathbf{B}^T \cdot \mathbf{A}^T\mathbf{B}[\mathbf{B}^T\mathbf{B}]^{-\frac{1}{2}}\right) \\
&\leq \rho\left([\mathbf{B}^T\mathbf{B}]^{-\frac{1}{2}}\mathbf{B}^T\mathbf{A}\mathbf{A}^T\mathbf{B}[\mathbf{B}^T\mathbf{B}]^{-\frac{1}{2}}\right) \\
&= \rho\left([\mathbf{B}^T\mathbf{B}]^{-1}\mathbf{B}^T\mathbf{A}\mathbf{A}^T\mathbf{B}\right) \\
&= \rho\left([\mathbf{B}^T\mathbf{A}\mathbf{A}^T\mathbf{B} + \mathbf{B}^T[I - \mathbf{A}\mathbf{A}^T]\mathbf{B}]^{-1}\mathbf{B}^T\mathbf{A}\mathbf{A}^T\mathbf{B}\right) \\
&< 1
\end{aligned}
$$

where the last inequality follows directly from Lemma 3. The inequality on the third line follows from the fact that the symmtric idempotent matrix $\mathbf{B}[\mathbf{B}^T\mathbf{B}]^{-1}\mathbf{B}^T$ satisfies: $0 \leq \mathbf{B}[\mathbf{B}^T\mathbf{B}]^{-1}\mathbf{B}^T \leq \mathbf{I}$. $\square$

B. PET ML-EM Results

Lemma 5 *Let the p-element vectors $\underline{P}_{d|*}$, $d = 1, \ldots, m$, span $\mathbb{R}^p$ and assume $m \geq p$. Assume that $\theta_b > 0$ for all $b = 1, \ldots, p$ and $\mathbf{Y}_d > 0$ for all $d = 1, \ldots, m$. Define the matrices:*

$$\mathbf{B} \stackrel{\text{def}}{=} \sum_{d=1}^{m} \mathbf{Y}_d \text{diag}_b\left(\frac{1}{\mu_d}\right) \underline{P}_{d|*} \underline{P}_{d|*}^T \text{diag}_b\left(\frac{1}{\mu_d}\right), \tag{75}$$

and

$$\mathbf{B} + \mathbf{C} \stackrel{\text{def}}{=} \text{diag}_b\left(\frac{1}{\theta_b} \sum_{d=1}^{m} \frac{\mathbf{Y}_d P_{d|b}}{\mu_d}\right), \tag{76}$$

where $\mu_d = \sum_{k=1}^{p} \theta_k P_{k|d}$. Then $\rho\left([\mathbf{B}+\mathbf{C}]^{-1}\mathbf{C}\right) \leq \alpha_1^2$ where $\alpha_1^2 \in [0, 1)$.

Proof

Since the $\underline{P}_{d|*}$'s span $\mathbb{R}^p$ and the $\mathbf{Y}_d$'s are positive the matrix $\mathbf{B}$ is positive definite. Hence, by Lemma 3, it will suffice to show that $\mathbf{C}$ is non-negative definite. Define $\mathbf{D} = \text{diag}_b(\theta_b)$. Then:

$$\begin{aligned}
\mathbf{C} &= \text{diag}_b\left(\frac{1}{\theta_b} \sum_{d=1}^{m} \frac{\mathbf{Y}_d P_{d|b}}{\mu_d}\right) - \sum_{d=1}^{m} \mathbf{Y}_d \text{diag}_b\left(\frac{1}{\mu_d}\right) \underline{P}_{d|*} \underline{P}_{d|*}^T \text{diag}_b\left(\frac{1}{\mu_d}\right) \\
&= \mathbf{D}^{-1}\left[\sum_{d=1}^{m} \mathbf{Y}_d \mathbf{E}_d\right] \mathbf{D}^{-1}
\end{aligned}$$

where

$$\mathbf{E}_d \stackrel{\text{def}}{=} \left\{\text{diag}_b\left(\frac{P_{d|b}\theta_b}{\mu_d}\right) - \text{diag}_b\left(\frac{\theta_b}{\mu_d}\right) \underline{P}_{d|*} \underline{P}_{d|*}^T \text{diag}_b\left(\frac{\theta_b}{\mu_d}\right)\right\} \tag{77}$$

Therefore it suffices to show that $\mathbf{E}_d \geq 0$ for all $d = 1, \ldots, m$. Let $u \in \mathbb{R}^p$ be arbitrary. Then

$$\begin{aligned}
u^T \mathbf{E} u &= \sum_{b=1}^{p} u_b^2 \frac{P_{d|b}\theta_b}{\mu_d} - \left(\sum_{b=1}^{p} u_b \frac{P_{d|b}\theta_b}{\mu_d}\right)^2 \\
&= \sum_{b=1}^{p} \frac{P_{d|b}\theta_b}{\mu_d} (u_b - \overline{u})^2 \\
&\geq 0
\end{aligned}$$

where $\overline{u} \stackrel{\text{def}}{=} \sum_{b=1}^{p} u_b \frac{P_{d|b}\theta_b}{\mu_d}$ and we have used the fact that $\sum_{b=1}^{p} \frac{P_{d|b}\theta_b}{\mu_d} = 1$. $\square$

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List of Figures

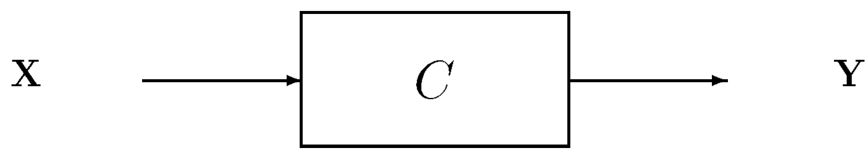

Figure 1: *A representation for* $\mathbf{Y}$ *as the output of a possibly noisy channel* C *with input* $\mathbf{X}$