Maximum Entropy on the Mean and the Cramér Rate Function in Statistical Estimation and Inverse Problems: Properties, Models, and Algorithms*

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Abstract. We explore a method of statistical estimation called *Maximum Entropy on the Mean* (MEM) which is based on an information-driven criterion that quantifies the compliance of a given point with a reference prior probability measure. At the core of this approach lies the *MEM function* which is a partial minimization of the Kullback-Leibler divergence over a linear constraint. In many cases, it is known that this function admits a simpler representation (known as the *Cramér rate function*). Via the connection to exponential families of probability distributions, we study general conditions under which this representation holds. We then address how the associated *MEM estimator* gives rise to a wide class of MEM-based regularized linear models for solving inverse problems. Finally, we propose an algorithmic framework to solve these problems efficiently based on the Bregman proximal gradient method, alongside proximal operators for commonly used reference distributions. The article is complemented by a software package for experimentation and exploration of the MEM approach in applications.

Key words. Maximum Entropy on the Mean, Statistical Estimation, Cramér Rate Function, Kullback-Leibler Divergence, Prior Distribution, Regularization, Linear Inverse Problems, Bregman Proximal Gradient, Convex Duality, Large Deviations.

MSC codes. 49M27, 29M29, 60F10, 62B10, 62H12, 90C25, 90C46

1. Introduction.

Many models for modern applications in various disciplines are based on some form of *statistical estimation*, for example the very common *maximum likelihood (ML)* principle. In this study, we consider an alternative approach known as the *maximum entropy on the mean* (MEM). At its core lies the MEM function κ_P induced by some *reference distribution* P and defined as

$$\kappa_P(y) := \inf \left\{ \mathrm{KL}(Q|P) : \mathbb{E}_Q = y, Q \in \mathcal{P}(\Omega) \right\},$$

where $P(\Omega)$ stands for the set of probability measures on $\Omega \subseteq \mathbb{R}^d$, $\mathbb{E}_Q$ is the expected value of $Q \in P(\Omega)$ and $\mathrm{KL}(Q|P)$ stands for the Kullback-Leibler (KL) divergence of Q with respect to P [38] (see Section 2 for precise definitions). Thus, the MEM modeling paradigm stems from the principle of minimum discrimination information [37] which generalizes the well-known principal of maximum entropy [36]. In the context of information theory [24], the argmin of $\kappa_P(y)$ is often referred to as the *information projection* of P onto the set $\{Q \in P(\Omega) : \mathbb{E}_Q = y\}$, the *closest* member of the set to P.

Various forms and interpretations of MEM have been studied (see for example, [26, 30, 31, 32, 34, 39, 40]) and found applications in various disciplines, including earth sciences [29, 42, 43, 45, 52], and medical imaging [1, 19, 22, 33, 35]. A version of the MEM method

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was recently explored for blind deblurring of images possessing some form of fixed symbology (for example, in barcodes) [47, 46]. There one exploited the ability of of the MEM framework to facilitate the incorporation of nonlinear constraints via the introduction of a prior distribution.

Despite its many interesting properties in both theory and applications, the MEM methodology has yet to find its place as a mainstream tool for statistical estimation, particularly as it pertains to solving inverse problems. One factor that might have contributed to this centers on the practical issue that there are no dedicated optimization algorithms designed to tackle models based on the MEM methodology. Indeed, the MEM function is defined by means of an infinite-dimensional optimization problem. Previous attempts to solve models involving the MEM function relied on its finite-dimensional dual problem. To the best of the authors' knowledge, there are no dedicated optimization algorithms designed to tackle models based on the MEM methodology. Therefore, any researcher or practitioner wishing to employ the MEM framework must first overcome a notable barrier of deriving an appropriate optimization algorithm for its solution. In this work, our goal is to fill in this gap, providing an accessible gate to the MEM methodology.

Our approach is based on the fundamental work by Brown [18, Chapter 6] and complements [39] by first proving the equivalence of the MEM function to the *Cramér's rate* function, mostly known from its role in *large deviation theory*. Cramér's rate function is defined by means of a finite-dimensional optimization problem as it is simply the convex conjugate of the log-normalizer (aka the comulant generating function) of the reference distribution P. In many cases (i.e., choices of P) it admits a closed form expression while in others it can still be evaluated efficiently. The connection between these seemingly different functions is well established in the large deviations [27], statistics [18], and information theory [39] literature. Nonetheless, various assumptions imposed in the aforementioned works limit the scope of existing results. Employing the framework of exponential families of probability distributions [18], we establish the equivalence between the two functions under very mild and natural conditions, allowing us to cover many distributions of practical interest. Thus, models involving MEM functions can be explicitly stated using the corresponding Cramér functions.

Central to our study is *the MEM estimator* which is shown to be well defined under very mild conditions. We further recall an insightful connection between the MEM and ML estimators as presented in [18] for the case of a reference distribution from an exponential family. As with the ML counterpart, the MEM estimator has vast applications, and hence we restrict the remainder of the paper to a wide class of regularized linear models for solving inverse problems. Each model in this class involves two MEM functions, one in the role of a fidelity term and another as a regularizer (comparable to the *maximum a priori (MAP) estimation* framework which extends ML). Let us provide an example: given a measurement matrix $A \in \mathbb{R}^{m\times d}$, an observation vector $\hat{y} \in \mathbb{R}^m$ and an additional vector $p \in [0,1]^d$ representing some prior knowledge, the following optimization problem

$$\min \left\{ \underbrace{\frac{1}{2}\|Ax-\hat{y}\|_2^2}_{Fidelity} + \underbrace{\sum_{i=1}^{d}\left[x_i \log\left(\frac{x_i}{p_i}\right) + (1-x_i)\log\left(\frac{1-x_i}{1-p_i}\right)\right]}_{Regularization} : x \in [0,1]^d \right\},$$

fits the MEM framework with normal (Gaussian) and Bernoulli reference distributions of the fidelity and regularization terms, respectively. Other choices of reference distributions will lead to additional models that admit similar additive composite structure. Moreover, the closed form expressions of the two functions in our example follow from the definition of Cramér's rate function. In models of these forms, concrete expressions and structures with distinct geometry can be exploited to customize appropriate optimization strategies. Here we highlight the class of *Bregman proximal gradient* (BPG) methods as an especially suitable choice for this family of models. Nevertheless, other methods are also viable alternatives; for example, adaptive and scaled, accelerated variants and dual decomposition methods which are defined by means of the same operators developed here.

Our overall aim is to provide a self-contained, mathematically sound toolbox for working with the MEM methodology for a wide variety of models. For this reason, we provide a comprehensive list of Cramér functions and operators used in the algorithms, and complement it with a software package. We believe this sets the basis for (and hopefully triggers) further experimentation and exploration of the MEM approach in contemporary applications.

The paper is organized as follows. In Section 2, we recall some concepts and preliminary results from convex analysis and probability theory which will be used in this work. In Section 3, we study the MEM and Cramér rate functions and establish the equivalence between the two under very mild and natural conditions. This allows us to use the accessible definition of the Cramér function and derive tractable expressions for a wide class of possible reference distributions which closes this section (see Table 1). Section 4 is devoted to the MEM models considered in this work, and in Section 5, we present the algorithms for solving such models. We end with a few concrete examples of problems and corresponding algorithms crafted from the operators derived in this work. An appendix provides deferred proofs and the details of a variety of Cramér rate function computations.

2. Preliminaries.

2.1. Convex Analysis.

We recall here some definitions and results from convex analysis. Further details and proofs can be found in various textbooks such as [9, 11, 48].

The *affine hull* of a set $S \subseteq \mathbb{R}^d$ is the smallest affine subspace containing S. For any point $y \in S$, we have the following relation

$$\operatorname{aff} S = y + \operatorname{span}(S - y), \tag{2.1}$$

where $\operatorname{span} S$ stands for the linear hull of S.The dimension of $\operatorname{aff} S$ is defined as $\dim(\operatorname{aff} S) := \dim(\operatorname{span}(S - y))$. The interior, closure and boundary of a set are denoted as $\operatorname{int} S$, $\operatorname{cl} S$ and $\operatorname{bd} S$, respectively.

The (Fenchel) conjugate of $\psi : \mathbb{R}^d \to [-\infty, \infty]$ is defined as

$$\psi^*(y) := \sup\{\langle y, x\rangle - \psi(x) : x \in \mathbb{R}^d\}.$$

The function ψ is proper if $\psi(x) > -\infty$ for all $x \in \mathbb{R}^d$ and $\operatorname{dom} \psi := \{x \in \mathbb{R}^d : \psi(x) < \infty\} \neq \emptyset$. In addition, ψ is closed, if its epigraph $\{(x, \alpha) \in \mathbb{R}^d \times \mathbb{R} : \psi(x) \leq \alpha\}$ is a closed set.

If ψ is proper and convex then ψ^* is closed, proper and convex. For a proper function $\psi : \mathbb{R}^d \to (-\infty, +\infty]$, the *Fenchel-Young inequality* states that $\psi(x) + \psi^*(y) \geq \langle y, x\rangle$. If ψ is proper, closed and convex then we obtain that [11, Theorem 4.20]

$$\psi(x) + \psi^*(y) = \langle y, x\rangle \iff y \in \partial\psi(x) \iff x \in \partial\psi^*(y), \tag{2.2}$$

where $\partial\psi(x) := \{g \in \mathbb{R}^d : \psi(y) \geq \psi(x) + \langle g, y - x\rangle \ (y \in \mathbb{R}^d)\}$ is the *subdifferential* of ψ at $x \in \mathbb{R}^d$.

The *indicator function* of a set $S \subseteq \mathbb{R}^d$ is denoted by δ_S and defined as $\delta_S(x) = 0$ if $x \in S$ and $\delta_S(x) = +\infty$ otherwise. Its convex conjugate is known as the *support function* $\sigma_S(y) := \delta_S^*(y) = \sup\{\langle y, x\rangle : x \in S\}$.

Definition 2.1 (Essential smoothness and Legendre type). *Let $\psi : \mathbb{R}^d \to (-\infty, +\infty]$ be proper and convex. Then, ψ is called* essentially smooth *if it satisfies the following conditions:*

1. $\operatorname{int}(\operatorname{dom}\psi) \neq \emptyset$*;*
2. ψ *is differentiable on* $\operatorname{int}(\operatorname{dom}\psi)$*;*
3. $\|\nabla\psi(x^k)\| \to \infty$ *for any sequence* $\{x^k \in \operatorname{int}(\operatorname{dom}\psi)\}_{k\in\mathbb{N}} \to \bar{x} \in \operatorname{bd}(\operatorname{dom}\psi)$*.*

The last condition listed above is called steepness*. An essentially smooth function ψ is said to be of* Legendre type *if it is strictly convex on* $\operatorname{int}(\operatorname{dom}\psi)$*.*

For $\psi : \mathbb{R}^d \to (-\infty, +\infty]$ closed and of Legendre type, the following hold [48, Theorem 26.5]:

1. ψ^* is of Legendre type.
2. $\nabla\psi : \operatorname{int}(\operatorname{dom}\psi) \to \operatorname{int}(\operatorname{dom}\psi^*)$ is a bijection with $(\nabla\psi)^{-1} = \nabla\psi^*$.

The *Bregman distance* induced by a function ψ of Legendre type is defined as [17]

$$D_\psi(y, x) = \psi(y) - \psi(x) - \langle\nabla\psi(x), y - x\rangle \qquad (x \in \operatorname{int}(\operatorname{dom}\psi), y \in \operatorname{dom}\psi).$$

For any $(x, y) \in \operatorname{int}(\operatorname{dom}\psi) \times \operatorname{dom}\psi$, the Bregman distance is nonnegative $D_\psi(y, x) \geq 0$, and equality holds if and only if $x = y$ due to strict convexity of ψ [17]. However, in general, D_ψ is not symmetric, unless $\psi = (1/2)\|\cdot\|^2$ [7, Lemma 3.16]. The Bregman distance induced by a function ψ of Legendre type satisfies the following additional properties [8, Theorem 3.7]: For any $x, y \in \operatorname{int}(\operatorname{dom}\psi)$ it holds that

$$D_\psi(y, x) = D_{\psi^*}(\nabla\psi(x), \nabla\psi(y)). \tag{2.3}$$

The Bregman distance is strictly convex with respect to its first argument. Moreover, for two functions ψ_1 and ψ_2 differentiable at $x \in \operatorname{int}(\operatorname{dom}\psi_1) \cap \operatorname{int}(\operatorname{dom}\psi_2)$

$$D_{\alpha\psi_1+\beta\psi_2}(y, x) = \alpha D_{\psi_1}(y, x) + \beta D_{\psi_2}(y, x) \quad (y \in \operatorname{dom}\psi_1 \cap \operatorname{dom}\psi_2,\ \alpha, \beta \in \mathbb{R}). \tag{2.4}$$

2.2. Probability Theory and Exponential Families. We recall some concepts from probability theory with an emphasis on exponential families. For further detail, see e.g. [4, 18].

Let $\mathcal{M}(\Omega)$ be the set of σ-finite measures defined over a measurable space (Ω, Σ) where $\Omega \subseteq \mathbb{R}^d$ and Σ is a σ*-algebra* on Ω. The *support* of ρ, namely the minimal closed measurable set $A \in \Sigma$ such that $\rho(\Omega \setminus A) = 0$, is denoted by Ω_ρ. We denote by $\Omega_\rho^{cc} := \operatorname{cl}(\operatorname{conv}\Omega_\rho)$ the closure of the convex hull of the support Ω_ρ, which is known as the *convex support* of ρ. Recall further that, if μ is another measure defined over (Ω, Σ), then μ is *absolutely continuous* with respect to ρ (denoted by $\mu \ll \rho$) if for every $A \in \Sigma$ such that $\rho(A) = 0$ it holds that $\mu(A) = 0$. In this case, the *Radon-Nikodym derivative* is the unique function $h = \frac{d\mu}{d\rho}$ such that

$\mu(A) = \int_A h d\rho$ for any $A \in \Sigma$. For a measurable space (Ω, Σ) we denote by $\nu \in \mathcal{M}(\Omega)$ the *dominating measure*. Throughout, we restrict ourselves to two scenarios: either $\Omega = \mathbb{R}^d$ and ν is the Lebesgue measure or Ω is a countable subset of $\mathbb{R}^d$ and ν is the counting measure. Let $\mathcal{P}(\Omega)$ be the set of probability measures defined over Ω and absolutely continuous with respect to ν. We emphasize that for $P \in \mathcal{P}(\Omega)$ the support Ω_P might be a proper subset of Ω, and thus there is no loss of generality in our setting even when $\Omega = \mathbb{R}^d$. Furthermore, for any set $A \subseteq \mathbb{R}^d$ the expression $P(A)$ should be understood as $P(A \cap \Omega)$. For $P \in \mathcal{P}(\Omega)$, the Radon-Nikodym derivative $f_P := \frac{dP}{d\nu}$ is either a probability density or mass function, depending on the set Ω. In both cases, we will refer to f_P as the density of the distribution.[1] The *expected value* (if it exists) and *moment generating function* of $P \in \mathcal{P}(\Omega)$ are given by

$$\mathbb{E}_P := \int_\Omega y dP(y) \in \mathbb{R}^d \qquad \text{and} \qquad M_P[\theta] := \int_\Omega \exp(\langle \cdot, \theta \rangle) dP,$$

respectively. For $P \in \mathcal{M}(\Omega)$ absolutely continuous with respect to ν, we define

$$\Theta_P := \left\{ \theta \in \mathbb{R}^d : \int_\Omega \exp(\langle \cdot, \theta \rangle) dP < \infty \right\},$$

and consider the function $\psi_P : \mathbb{R}^d \to (-\infty, +\infty]$ given by

$$\psi_P(\theta) := \begin{cases} \log \int_\Omega \exp\left(\langle \cdot, \theta \rangle\right) dP, & \theta \in \Theta_P, \\ +\infty, & \theta \notin \Theta_P. \end{cases} \tag{2.5}$$

Then $\mathcal{F}_P := \{ f_{P_\theta}(y) := \exp\left(\langle y, \theta \rangle - \psi_P(\theta)\right) : \theta \in \Theta_P \}$, is a *standard exponential family* generated by P. Note that, the probability measure P_θ satisfying $dP_\theta = f_{P_\theta} dP$ is, by construction, a probability measure such that P_θ and P are mutually absolutely continuous, hence $\Omega_{P_\theta} = \Omega_P$ for all $\theta \in \Theta_P$ [4, Section 8.1]. The function ψ_P is called the *log-normalizer* (also known as the *log-partition* or *log-Laplace transform* of P). The vector $\theta \in \mathbb{R}^d$ is known as the *natural parameter* and the set $\Theta_P = \operatorname{dom} \psi_P$ is called the *natural parameter space*.[2]

The following results summarize some well-known properties of the log-normalizer ψ_P.

Proposition 2.2 (Convexity, [18, Theorem 1.13]). *Let $\mathcal{F}_P$ be an exponential family generated by $P \in \mathcal{M}(\Omega)$. Then, the natural parameter space Θ_P is a convex set and the log-normalizer function $\psi_P : \mathbb{R}^d \to (-\infty, +\infty]$ is closed, proper and convex.*

Proposition 2.3 (Differentiability, [18, Theorem 2.2, Corollary 2.3]). *Let $\mathcal{F}_P$ be an exponential family generated by $P \in \mathcal{M}(\Omega)$ and let $\theta \in \operatorname{int} \Theta_P$. Then, the log normalizer $\psi_P : \mathbb{R}^d \to (-\infty, +\infty]$ is infinitely differentiable at θ and it holds that $\nabla \psi_P(\theta) = \mathbb{E}_{P_\theta}$.*

The dimension of a convex set $S \subseteq \mathbb{R}^d$, denoted by $\dim S$, is equal to the affine dimension of $\operatorname{aff} S$. We assume that the exponential family generated by $P \in \mathcal{M}(\Omega)$ is *minimal*, i.e., $\dim \Theta_P = \dim \Omega_P^{cc} = d$ or, equivalently, $\operatorname{int} \Theta_P \neq \emptyset$ and $\operatorname{int} \Omega_P^{cc} \neq \emptyset$. This is not restrictive as a non-minimal exponential family can be always reduced to a minimal form [18, Theorem 1.9]. The following result strengthens Proposition 2.2 for minimal exponential families.

[1] We will interchangeably refer to $P \in \mathcal{P}(\Omega)$ as either a distribution or measure.

[2] It is possible to define the exponential family $\mathcal{F}_P$ over a subset of the natural parameter space [18, Definition 1.1], but this is not needed for our study.

Proposition 2.4 (Strict convexity, [18, Theorem 1.13]). *Let $\mathcal{F}_P$ be a minimal exponential family generated by $P \in \mathcal{M}(\Omega)$. Then, the log-normalizer function $\psi_P : \mathbb{R}^d \to (-\infty, +\infty]$ is strictly convex over Θ_P.*

If the log-normalizer ψ_P is essentially smooth (or 'steep' in the exponential family terminology, see, e.g., [4, Theorem 5.27] and [18, Definition 3.2]), we say that the exponential family $\mathcal{F}_P$ is *steep*. This condition is automatically satisfied when Θ_P is open [4, Theorem 8.2]. While most exponential families encountered in practice have this property, there are relevant cases when this assumption is too restrictive (e.g., [18, Example 3.4]). Thus, in order to cover all examples provided in this work, we will assume that the exponential family is steep. Summarizing the above discussion and recalling Definition 2.1 we have the following corollary.

Corollary 2.5. *Let $\mathcal{F}_P$ be a minimal and steep exponential family generated by $P \in \mathcal{M}(\Omega)$. Then, the log normalizer function ψ_P is of Legendre type.*

From the last corollary we can see that $\nabla\psi_P$ forms a bijection between $\operatorname{int}(\operatorname{dom}\psi_P) = \operatorname{int}\Theta_P$ and $\operatorname{int}(\operatorname{dom}\psi_P^*)$. This relation, provides a dual representation of the log-normalizer ψ_P and, consequently, the distribution in question. The so-called *mean value parametrization* is obtained by applying a change of variables where the natural parameter θ is replaced by $\mu \in \mathbb{R}^d$ such that $\mu = \mathbb{E}_{P_\theta} = \nabla\psi_P(\theta)$, i.e., $\theta = \nabla\psi_P^*(\mu)$.

The *Kullback-Leibler (KL) divergence* (also known as the relative entropy) of a probability measure $Q \in \mathcal{P}(\Omega)$ with respect to $P \in \mathcal{P}(\Omega)$ is given by (see [38])

$$\mathrm{KL}(Q|P) := \begin{cases} \displaystyle\int_\Omega \log\left(\frac{dQ}{dP}\right) dQ, & Q \ll P, \\ +\infty, & \text{otherwise.} \end{cases}$$

It holds that $\mathrm{KL}(Q|P) \geq 0$ with equality if and only if $Q = P$ [38, Lemma 3.1]. Thus, the Kullback-Leibler information quantifies the dissimilarity between two probability measures. We note that, in general, $\mathrm{KL}(Q|P)$ is not symmetric. Furthermore, $\mathrm{KL}(Q|P)$ is jointly convex in $(Q|P)$. We record a special case for which the KL divergence is of particular interest.

Remark 2.6 (Kullback-Leibler divergence for exponential family). Let $\mathcal{F}_P$ be an exponential family generated by $P \in \mathcal{M}(\Omega)$. Let $\theta_1 \in \Theta_P$ and $\theta_2 \in \operatorname{int}\Theta_P$, thus for $i = 1, 2$ we have that $f_{P_{\theta_i}} \in \mathcal{F}_P$. In this case, the KL divergence between the two measures $P_{\theta_i} \in \mathcal{P}(\Omega)$ such that $dP_{\theta_i} := f_{P_{\theta_i}} dP$ $(i = 1, 2)$ satisfies $\mathrm{KL}(P_{\theta_2}|P_{\theta_1}) = D_{\psi_P}(\theta_1, \theta_2)$ [18, Proposition 6.3]. ◊

3. Maximum entropy on the mean and Cramér's rate function.

For $y \in \mathbb{R}^d$, the density

$$f_P(y) := \frac{dP}{d\nu}(y) \tag{3.1}$$

provides an indication of the likelihood of y under the distribution $P \in \mathcal{P}(\Omega)$. The method of *Maximum Entropy on the Mean* (MEM) suggests an alternative, information driven function $\kappa_P : \mathbb{R}^d \to (-\infty, +\infty]$ given by

$$\kappa_P(y) := \inf\left\{\mathrm{KL}(Q|P) : \mathbb{E}_Q = y, Q \in \mathcal{P}(\Omega)\right\}. \tag{3.2}$$

Here, κ_P measures how y complies with the distribution P, by seeking a distribution Q with expected value y that minimizes $\mathrm{KL}(\cdot|P)$. The distance, in terms of the KL divergence (the information gain) between the resulting and the original distributions quantifies the compliance of y with P. We will refer to κ_P as the *MEM function* and to P as the *reference distribution*. Since $\mathrm{KL}(Q|P) \geq 0$ and $\mathrm{KL}(Q|P) = 0$ if and only if $Q = P$, we find that the MEM function satisfies $\kappa_P(y) \geq 0$ for any $y \in \mathbb{R}^d$ and $\kappa_P(y) = 0$ if and only if $y = \mathbb{E}_P$.

In most cases of interest, the MEM function admits an alternative representation which sheds light on many of its additional properties (cf. Theorem 3.10). More precisely, under suitable conditions (cf. Theorem 3.8), the MEM function coincides with the *Cramér rate function* [25], to which we turn now. For a given reference distribution $P \in \mathcal{P}(\Omega)$, recall the log-nomalizer previously defined for a general measure in (2.5):

$$\psi_P(\theta) := \log M_P[\theta] = \log \int_\Omega \exp\left(\langle \cdot, \theta\rangle\right) dP.$$

In the context of probability measures P, ψ_P is often known as the *cumulant generating function*. The *Cramér rate function* ψ_P^* associated with P is the conjugate of ψ_P, that is,

$$\psi_P^*(y) \;=\; \sup\{\langle y, \theta\rangle - \psi_P(\theta) : \theta \in \mathbb{R}^d\}.$$

Our central assumption (which is not too restrictive in view of our discussion above) on the prior P and its exponential family $\mathcal{F}_P$ is provided below. The additional condition $0 \in \operatorname{int}\Theta_P$ insures the existence of $\mathbb{E}_P$.

Assumption 3.1. *The reference distribution $P \in \mathcal{P}(\Omega)$ generates a minimal and steep exponential family $\mathcal{F}_P$ such that $0 \in \operatorname{int}\Theta_P$.*

The equivalence between the two seemingly different functions[3] ψ_P^* and κ_P was previously established under various assumptions: the authors of [27, Theorem 5.2] (see also [28]) impose the (restrictive) assumption that ψ_P is finite. On the other hand, the results in [18, Theorem 6.17] and [39, Proposition 1] (see also [13] and a closely related result in [54, Theorem 3.4]) do not address the challenging case when y resides on the boundary of the domain. This scenario turns out to be important if (and only if) the reference distribution is defined over a countable set. Here, we provide a complete proof that overcomes these assumptions previously imposed. Our approach emphasizes the role played by the convex support of the reference distribution and leads to natural and easy to verify conditions. To this end, we will first need to examine the domains $\operatorname{dom}\kappa_P$ and $\operatorname{dom}\psi_P^*$. For Cramér's rate function ψ_P^*, a characterization of the domain is summarized in the following proposition.

Proposition 3.2 (Domain of the Cramér rate function ψ_P^* [4, Theorems 9.1, 9.4 and 9.5]). *Let $P \in \mathcal{P}(\Omega)$ be a reference distribution satisfying Assumption 3.1. Then,* $\operatorname{int}\Omega_P^{cc} \subseteq \operatorname{dom}\psi_P^* \subseteq \Omega_P^{cc}$. *Moreover, the following hold:*

(a) If Ω_P is finite, then $\operatorname{dom}\psi_P^* = \Omega_P^{cc}$.
(b) If Ω_P is countable, then $\operatorname{dom}\psi_P^* \supseteq \operatorname{conv}\Omega_P$.
(c) If Ω_P is uncountable, then $\operatorname{dom}\psi_P^* = \operatorname{int}\Omega_P^{cc}$.

[3] ψ_P^* appears in *Cramér's Theorem* central in large deviations theory [28]. A more general form of κ_P appears in *Sanov's Theorem*.

In order to establish a similar characterization for the domain of the MEM function, we will need to make precise the relation between Ω_P and the expected value $\mathbb{E}_P$ for a given probability measure $P \in \mathcal{P}(\Omega)$. To this end, we first recall some additional definitions and results (see, for example, [48, Section 6]). Consider two subsets $S, \hat{S} \subseteq \mathbb{R}^d$ and assume further that $S \subseteq \hat{S}$. Then $\operatorname{cl} S \subseteq \operatorname{cl} \hat{S}, \operatorname{int} S \subseteq \operatorname{int} \hat{S}$ and $\operatorname{conv} S \subseteq \operatorname{conv} \hat{S}$.

Denote the closed Euclidean unit ball in $\mathbb{R}^d$ by $\mathcal{B}_d$. The *relative interior* [48, Section 6] of a convex set $S \subseteq \mathbb{R}^d$ is defined as

$$\operatorname{ri} S := \Big\{ x \in \mathbb{R}^d : \exists \tau > 0 \text{ such that } (x + \tau \mathcal{B}_d) \cap \operatorname{aff} S \subseteq S \Big\}.$$

E.g., for the *unit simplex* $\Delta_d := \{y \in \mathbb{R}^d_+ : \langle e, y\rangle = 1\}$ we have $\operatorname{ri} \Delta_d := \{y \in \mathbb{R}^d_{++} : \langle e, y\rangle = 1\}$. Some facts which will be used in the sequel are summarized in the following lemma. Further details and proofs can be found in [48, Section 6, Theorem 13.1].

Lemma 3.3 (On the relative interior). *Let $S \subseteq \mathbb{R}^d$ be nonempty and convex. Then:*
(a) It holds that $\operatorname{ri}(\operatorname{cl} S) = \operatorname{ri} S$ and $\operatorname{ri} S \subseteq S \subseteq \operatorname{cl} S$.
(b) If $\dim S = d$ then $\operatorname{ri} S = \operatorname{int} S$ and, in particular, $\operatorname{int} S \neq \emptyset$.
(c) It holds that $x \in \operatorname{ri} S$ if and only if $\sigma_{S-x}(v) \geq 0$ where the last inequality is strict for every $v \in \mathbb{R}^d$ such that $-\sigma_S(-v) \neq \sigma_S(v)$.

Lemma 3.4 (Domain of expected value). *Let $P \in \mathcal{P}(\Omega)$ and assume that $\mathbb{E}_P$ exists. Then $\mathbb{E}_P \in \operatorname{ri} \Omega_P^{cc} = \operatorname{ri}(\operatorname{conv} \Omega_P)$.*

Proof. By definition of σ_{Ω_P}, for any $v \in \mathbb{R}^d$, it holds that $-\sigma_{\Omega_P}(-v) \leq \langle v, y\rangle \leq \sigma_{\Omega_P}(v)$. As $P \in \mathcal{P}(\Omega)$, this implies, for all $v \in \mathbb{R}^d$, that

$$\langle v, \mathbb{E}_P\rangle = \int_{\Omega_P} \langle v, y\rangle dP(y) \leq \sigma_{\Omega_P}(v) \int_{\Omega_P} dP(y) = \sigma_{\Omega_P}(v). \tag{3.3}$$

If there exists some subset $A \subseteq \Omega_P$ such that $P(\{y \in A : \langle v, y\rangle < \sigma_{\Omega_P}(v)\}) > 0$, then the inequality in (3.3) is strict. We will show that, for any $v \in \mathbb{R}^d$ such that $-\sigma_{\Omega_P}(-v) \neq \sigma_{\Omega_P}(v)$, such a subset exists; the desired result then follows from Lemma 3.3 (c) and the equivalence $\sigma_{\Omega_P^{cc}}(v) = \sigma_{\Omega_P}(v)$ [49, Theorem 8.24]. Indeed, let $v \in \mathbb{R}^d$ such that $-\sigma_{\Omega_P}(-v) \neq \sigma_{\Omega_P}(v)$, i.e. $-\sigma_{\Omega_P}(-v) < \sigma_{\Omega_P}(v)$. Pick $\tau \in (-\sigma_{\Omega_P}(-v), \sigma_{\Omega_P}(v))$ and consider $A = \{y \in \Omega_P : \langle v, y\rangle \leq \tau\}$. As $\tau < \sigma_{\Omega_P}(v)$, we have $A \subset \{y \in \Omega_P : \langle v, y\rangle < \sigma_{\Omega_P}(v)\}$, and

$$P(A) = P(\{y \in \Omega_P : \langle -v, y\rangle \geq -\tau\}) = P(\{y \in \Omega_P : \sigma_{\Omega_P}(-v) \geq \langle -v, y\rangle \geq -\tau\}) > 0,$$

where the strict inequality follows from the definition of $\sigma_{\Omega_P}(-v)$ and $\sigma_{\Omega_P}(-v) > -\tau$. Hence, A satisfies the desired conditions, which establishes the result. ■

We are now in a position to present and prove a characterization for the domain of the MEM function, analogous to Proposition 3.2. We will use the following notation

$$\mathcal{Q}_P(y) := \{Q \in \mathcal{P}(\Omega) : \mathbb{E}_Q = y,\ Q \ll P\}.$$

Observe that $y \in \operatorname{dom} \kappa_P$ if and only if $\mathcal{Q}_P(y) \neq \emptyset$.

Lemma 3.5 (Domain of the MEM function κ_P). *Let $P \in \mathcal{P}(\Omega)$ be a reference distribution satisfying Assumption 3.1. Then:*

(a) If Ω_P is countable, then $\operatorname{dom}\kappa_P = \operatorname{conv}\Omega_P$. *Hence, if Ω_P is finite, then* $\operatorname{dom}\kappa_P = \Omega_P^{cc}$.
(b) If Ω_P is uncountable, then $\operatorname{dom}\kappa_P = \operatorname{int}\Omega_P^{cc}$.

Proof. (a) Let $y \in \operatorname{dom}\kappa_P$, hence there exists $Q \in \mathcal{Q}_P(y)$. As $Q \ll P$, we obtain $\Omega_Q \subseteq \Omega_P$, thus $\operatorname{conv}\Omega_Q \subseteq \operatorname{conv}\Omega_P$. Hence, by Lemma 3.3 (a) and Lemma 3.4, we know that $y = \mathbb{E}_Q \in \operatorname{ri}\Omega_Q^{cc} \subseteq \operatorname{conv}\Omega_Q \subseteq \operatorname{conv}\Omega_P$. Thus, $\operatorname{dom}\kappa_P \subseteq \operatorname{conv}\Omega_P$. For the converse inclusion, let $y \in \operatorname{conv}\Omega_P$. By Carathéodory's theorem [20], there exist $n \leq d+1$ points $p_1, \ldots, p_n$ in Ω_P such that $y = \sum_{i=1}^n \lambda_i p_i$ for some $\lambda \in \Delta_n$. Consider a distribution $Q \in \mathcal{P}(\Omega)$ satisfying $Q(\{p_i\}) = \lambda_i$ for all $i = 1, \ldots, n$. Then, $Q \in \mathcal{Q}_P(y)$ by construction. Thus, $y \in \operatorname{dom}\kappa_P$, and we can conclude that $\operatorname{conv}\Omega_P \subseteq \operatorname{dom}\kappa_P$.
(b) First, let $y \in \operatorname{dom}\kappa_P$, then there exists $Q \in \mathcal{Q}_P(y)$. Since $Q \ll P$ which satisfies Assumption 3.1, it holds that $\dim\Omega_Q^{cc} = \Omega_P^{cc} = d$. Otherwise, the probability measure Q ($Q(\Omega_Q) = 1$) is concentrated on a lower dimensional affine subspace in contradiction to the absolute continuity of Q with respect to P. Hence, using Lemma 3.4 and Lemma 3.3 (b), we obtain that $y = \mathbb{E}_Q \in \operatorname{ri}\Omega_Q^{cc} = \operatorname{int}\Omega_Q^{cc} \subseteq \operatorname{int}\Omega_P^{cc}$. For the converse inclusion, by Proposition 3.2, $y \in \operatorname{int}\Omega_P^{cc} = \operatorname{dom}\psi_P^* = \operatorname{int}(\operatorname{dom}\psi_P^*) = \operatorname{dom}\nabla\psi_P^*$, and we conclude that $y = \mathbb{E}_{P_\theta}$ for $\theta = \nabla\psi_P^*(y)$. Since $P_\theta \ll P$ for P_θ from the exponential family generated by P, we find that $P_\theta \in \mathcal{Q}_P(y)$ and therefore $y \in \operatorname{dom}\kappa_P$. ■

Combining Lemma 3.5 with Proposition 3.2 yields the following corollary.

Corollary 3.6. *Let $P \in \mathcal{P}(\Omega)$ be a reference distribution satisfying Assumption 3.1. Then,*
(a) If Ω_P is countable and $\operatorname{conv}\Omega_P$ is closed (i.e., $\operatorname{conv}\Omega_P = \Omega_P^{cc}$), then $\operatorname{dom}\kappa_P = \operatorname{dom}\psi_P^* = \Omega_P^{cc}$. In particular, $\operatorname{dom}\kappa_P = \operatorname{dom}\psi_P^* = \Omega_P^{cc}$ if Ω_P is finite.
(b) If Ω_P is uncountable, then $\operatorname{dom}\kappa_P = \operatorname{dom}\psi_P^* = \operatorname{int}\Omega_P^{cc}$.

The following lemma will be crucial for proving the equivalence between the MEM function κ_P and Cramér's rate function ψ_P^*. The proof of the lower bound follows similar arguments as in [18, Theorem 6.17] and [39, Proposition 1] and we include it here for completeness.

Lemma 3.7. *Let $P \in \mathcal{P}(\Omega)$ be a reference distribution satisfying Assumption 3.1. Then:*

$$\psi_P^*(y) \leq \kappa_P(y) \leq \psi_P^*(y) + KL(Q|P_\theta) - D_{\psi_P^*}(y, \nabla\psi_P(\theta)),$$

for any $y \in \operatorname{dom}\kappa_P$, $Q \in \mathcal{Q}_P(y)$ and $\theta \in \operatorname{int}\Theta_P$.

Proof. For any $\theta \in \operatorname{int}\Theta_P$ and $Q \in \mathcal{Q}_P(y)$ we obtain that $Q \ll P_\theta$ due to the mutual absolute continuity between P_θ and P. Hence,

$$\begin{aligned}(3.4)\quad \mathrm{KL}(Q|P) &= \int_\Omega \log\left(\frac{dQ}{dP}\right) dQ = \int_\Omega \log\left(\frac{dQ}{dP_\theta}\right) dQ + \int_\Omega \log\left(\frac{dP_\theta}{dP}\right) dQ \\ &= \mathrm{KL}(Q|P_\theta) + \int_\Omega [\langle z, \theta\rangle - \psi_P(\theta)] dQ(z) = \mathrm{KL}(Q|P_\theta) + \langle y, \theta\rangle - \psi_P(\theta),\end{aligned}$$

where the last identity uses $y = \mathbb{E}_Q$. Since (3.4) holds for all $\theta \in \operatorname{int}\Theta_P$ and $\mathrm{KL}(Q|P_\theta) \geq 0$,

$$(3.5)\qquad \mathrm{KL}(Q|P) \geq \sup\{\langle y, \theta\rangle - \psi_P(\theta) : \theta \in \operatorname{int}\Theta_P\} = \psi_P^*(y),$$

due to the closedness of ψ_P, see Proposition 2.2. The lower bound for κ_P follows immediately from its definition and the above inequality.

As for the upper bound: by (3.4) and (2.2), for any $Q \in \mathcal{Q}_P(y)$ and $\theta \in \operatorname{int}\Theta_P$, we have

$$\begin{aligned}\mathrm{KL}(Q|P) &= \mathrm{KL}(Q|P_\theta) + \langle y,\theta\rangle - \psi_P(\theta)\\ &= \mathrm{KL}(Q|P_\theta) + \langle y - \nabla\psi_P(\theta),\theta\rangle + \langle\nabla\psi_P(\theta),\theta\rangle - \psi_P(\theta)\\ &= \mathrm{KL}(Q|P_\theta) - [\psi_P^*(y) - \psi_P^*(\nabla\psi_P(\theta)) - \langle y-\nabla\psi_P(\theta),\theta\rangle] + \psi_P^*(y)\\ &= \mathrm{KL}(Q|P_\theta) - D_{\psi_P^*}(y,\nabla\psi_P(\theta)) + \psi_P^*(y).\end{aligned}$$

Then the result follows due to the fact that $\kappa_P(y) \le \mathrm{KL}(Q|P)$ for all $Q \in \mathcal{Q}_P(y)$. ■

Theorem 3.8 (Equivalence between Cramér's rate function and the MEM function). *Let $P \in \mathcal{P}(\Omega)$ satisfy Assumption 3.1, and assume that one of the following two conditions holds:*

(i) Ω_P is uncountable.

(ii) Ω_P is countable and $\operatorname{conv}\Omega_P$ is closed (as is the case when Ω_P is finite).

Then, $\kappa_P = \psi_P^*$. In particular, κ_P is closed, proper and convex.

Proof. First, let $y \in \operatorname{int}\Omega_P^{cc}$. By Assumption 3.1, $\nabla\psi_P$ is a bijection between $\operatorname{int}(\operatorname{dom}\psi_P)$ $= \operatorname{int}\Theta_P$ and $\operatorname{int}(\operatorname{dom}\psi_P^*) = \operatorname{int}\Omega_P^{cc}$, where the latter uses Proposition 3.2. Thus, there exists $\theta \in \operatorname{int}\Theta_P$ such that $y = \nabla\psi_P(\theta) = \mathbb{E}_{P_\theta}$. Applying Lemma 3.7 with $Q = P_\theta$ yields

$$\kappa_P(y) = \psi_P^*(y) \qquad (y \in \operatorname{int}\Omega_P^{cc}). \tag{3.6}$$

Due to Corollary 3.6, this establishes the result when Ω_P is uncountable. To complete the proof, we only need to address the case when $y \in \operatorname{bd}\Omega_P^{cc}$ under assumption (ii). By Corollary 3.6, in this case $\operatorname{dom}\kappa_P = \operatorname{dom}\psi_P^* = \Omega_P^{cc}$ and $\mathcal{Q}_P(y) \neq \emptyset$ for $y \in \operatorname{bd}\Omega_P^{cc}$. Consider any $Q \in \mathcal{Q}_P(y)$, then, by definition of κ_P, we have that

$$\kappa_P(y) \le \mathrm{KL}(Q|P) < +\infty. \tag{3.7}$$

Choose any $\hat{y} \in \operatorname{int}\Omega_P^{cc}$ and set $\hat\theta = \nabla\psi_P^*(\hat y)$ (i.e., $\hat y = \nabla\psi(\hat\theta)$). For any $\lambda \in [0,1)$ consider $Q_\lambda = \lambda Q + (1-\lambda)P_{\hat\theta}$. Then, by linearity of $Q \mapsto \mathbb{E}_Q$ [46, Lemma 2], we obtain

$$y_\lambda := \mathbb{E}_{Q_\lambda} = \lambda\mathbb{E}_Q + (1-\lambda)\mathbb{E}_{P_{\hat\theta}} = \lambda y + (1-\lambda)\hat y.$$

By convexity of Ω_P^{cc} and the line segment principle [10, Lemma 6.28] we conclude that $y_\lambda \in \operatorname{int}\Omega_P^{cc}$. Set $\theta_\lambda := \nabla\psi_P^*(y_\lambda)$ and observe that, by Lemma 3.7 and the nonnegativity of the Bregman distance, it holds that

$$\psi_P^*(y) \le \kappa_P(y) \le \psi_P^*(y) + \mathrm{KL}(Q|Q_\lambda). \tag{3.8}$$

In addition, due to (3.7) and the fact that $Q \ll P \ll P_{\hat\theta}$, we conclude that $\mathrm{KL}(Q|P_{\hat\theta}) < \infty$. Thus, by (3.8) and convexity of $\mathrm{KL}(Q|\cdot)$, we obtain

$$\mathrm{KL}(Q|Q_\lambda) \le \lambda\mathrm{KL}(Q|Q) + (1-\lambda)\mathrm{KL}(Q|P_{\hat\theta}) \to 0 \quad \text{as} \quad \lambda \to 1. \qquad ■$$

We refer to a solution of the optimization problem (3.2) as the *MEM distribution* and denote it as Q_{MEM}. By similar arguments to the ones used in order to establish the lower bound in

Lemma 3.7, one can show that, when $y \in \mathrm{int}(\mathrm{dom}\,\kappa_P) = \mathrm{int}(\mathrm{conv}\,\Omega_P)$, the MEM distribution is a particular member of the exponential family generated by the reference distribution P. More precisely, it holds that $Q_{MEM} = P_\theta$ where $\theta = \nabla\psi_P^*(y)$ and consequently

$$f_{Q_{MEM}}(x) = \frac{dP_\theta}{dP}(x) = \exp\left(\langle x, \theta\rangle - \log \int_\Omega \exp(\langle\cdot, \theta\rangle)dP\right) = \frac{\exp(\langle x, \theta\rangle)}{\int_\Omega \exp(\langle\cdot, \theta\rangle)dP}.$$

This, again, highlights the intimate connection between the MEM function and exponential families. The case $y \in \mathrm{bd}\,(\mathrm{dom}\,\kappa_P)$ is more subtle and will be the topic of future research.

In what follows, we assume that the reference distribution of the MEM function satisfies the conditions stated in Theorem 3.8, that is:

Assumption 3.9. *The distribution $P \in \mathcal{P}(\Omega)$ satisfies one of the following conditions:*
(i) Ω_P is uncountable.
(ii) Ω_P is countable and $\mathrm{conv}\,\Omega_P$ is closed (as is the case when Ω_P is finite).

Under Assumptions 3.1 and 3.9, the MEM function and the Cramér rate function coincide. As an immediate consequence, we obtain that the MEM function κ_P is of Legendre type. More importantly, we will see that the alternative representation by means of Cramér's rate function is more tractable compared to the original definition given in (3.2).

Theorem 3.10 (Properties of the MEM function). *Let $P \in \mathcal{P}(\Omega)$ satisfy Assumptions 3.1 and 3.9. Then the following hold:*
(a) $\kappa_P(y) \geq 0$ and equality holds if and only if $y = \mathbb{E}_P$.
(b) κ_P is of Legendre type.
(c) κ_P is coercive in the sense that $\lim_{\|y\|\to\infty} \kappa_P(y) = +\infty$ [9, Definition 11.10]. In particular, $\kappa_P(y)$ is level bounded.
(d) If M_P is finite (which holds, in particular, when Ω_P is bounded), then κ_P is supercoercive in the sense that $\lim_{\|y\|\to\infty} \kappa_P(y)/\|y\| = +\infty$ [9, Definition 11.10].

Proof. Part (a) is evident from the definition of κ_P as given in (3.2) and [18, Proposition 6.2]. Part (b) follows directly from the equivalence to the Cramér rate function ψ_P^* and Corollary 2.5. To see (c), observe that (a) implies that κ_P admits a unique minimizer $\mathbb{E}_P$ which combined with the fact that κ_P is closed, proper and convex (since κ_P is of Legendre type due to (b)) establishes the result by [2, Proposition 3.1.3]. Lastly, if the moment generating function is finite, then so is ψ_P, and the supercoercivity of $\kappa_P = \psi_P^*$ follows from [49, Theorem 11.8(d)].[4] If Ω_P is bounded then $\mathrm{dom}\,\kappa_P$ is bounded due to Lemma 3.5. In this case, $\kappa_P = \psi_P^*$ is trivially supercoercive and the claim that ψ_P is finite follows from [49, Theorem 11.8(d)]. ■

The results presented in the remainder of this work are established under Assumptions 3.1 and 3.9 which, in particular, ensure the equivalence between the MEM and Cramér rate functions. For this reason, we take this opportunity to standardize our nomenclature: between the two options (κ_P or ψ_P^*) we will opt for the one that corresponds to the Cramér rate function ψ_P^*. This choice is motivated by our intent to emphasize the more computationally appealing definition and the connection to the log-normalizer function ψ_P. Nevertheless, in the definition

[4] The definition of supercoercive convex functions we use here follows [9, Definition 11.10]. In [49] the authors refer to such functions as coercive (see [49, Definition 3.25]).

of some new concepts defined by means of Cramér's rate function, we will adopt the MEM terminology in order to emphasize the motivation in the context of estimation.

If the reference distribution belongs to an exponential family generated by some measure $P \in \mathcal{M}(\Omega)$, i.e., if for some $\hat{\theta} \in \Theta_P$ we consider a new exponential family generated by the probability measure $P_{\hat{\theta}}$,[5] then the corresponding moment generating function takes the form

$$M_{P_{\hat{\theta}}}[\theta] = \exp\left(\psi_P(\hat{\theta}+\theta) - \psi_P(\hat{\theta})\right). \tag{3.9}$$

In this case, the Cramér rate functions that corresponds to $P_{\hat{\theta}}$ and P share a useful relation summarized in the following lemma. We include the simple proof in Appendix A.

Lemma 3.11. *Let $\mathcal{F}_P$ be a minimal and steep exponential family generated by $P \in \mathcal{M}(\Omega)$ and assume further that, for any $\theta \in \operatorname{int}\Theta_P$, Assumption 3.9 holds for $P_\theta \in \mathcal{P}(\Omega)$. Then, for any $\hat{\theta} \in \operatorname{int}\Theta_P$ and $y \in \operatorname{dom}\psi_P^*$, we have $\psi^*_{P_{\hat{\theta}}}(y) = D_{\psi_P^*}(y,\hat{y})$ where $\hat{y} := \nabla\psi_P(\hat{\theta}) \in \operatorname{int}\Omega_P^{cc}$.*

We list in Table 1 below a number of examples of Cramér rate functions that correspond to most of the popular distributions (i.e. choices of the reference distribution $P \in \mathcal{P}(\Omega)$). Some of the functions admit a closed form expression while others are given implicitly.[6] The derivations and further details are included as a supplementary material. Observe that all cases considered below satisfy Assumptions 3.1 and 3.9 which guarantees the equivalence established in Theorem 3.8: indeed, with some exceptions, all the distributions in Table 1 are minimal with a natural parameter space Θ_P open which implies steepness. These exceptions are: the multinomial distribution which is minimal under an appropriate reformulation, and the multivariate normal-inverse Gaussian which is steep (see supplementary material). Here, we provide the Cramér rate function of the multinomial distribution in minimal form. Thus, Assumption 3.1 holds for all the distributions given in Table 1. This comprehensive list complements and extends some previously established formulas [39, 54].

Many computations are facilitated in the presence of separability as described in the following remark.

Remark 3.12 (Separability of ψ_P^*). In most examples, the reference distribution $P \in \mathcal{P}(\Omega)$ admits a separable structure of the form $P(y) = P_1(y_1)P_2(y_2)\cdots P_d(y_d)$ where $P_i \in \mathcal{P}(\Omega_i)$, $\Omega_i \subset \mathbb{R}$, i.e., each component corresponds to an i.i.d. random variable. In this case, since $\mathbb{M}_P[\theta] = \prod_{i=1}^d \mathbb{M}_{P_i}[\theta_i]$ [50, Section 4.4], we have

$$\psi_P^*(y) = \sup\left\{\langle y,\theta\rangle - \log\left(\mathbb{M}_P[\theta]\right) : \theta \in \mathbb{R}^d\right\} = \sum_{i=1}^d \sup\left\{y_i\theta_i - \log\left(\mathbb{M}_{P_i}[\theta_i]\right) : \theta_i \in \mathbb{R}\right\}.$$

Hence, in most of our examples below we will consider only the case $d = 1$. ♢

In Table 1 we employ the convention that $0\log(0) = 0$ and define

$$\Delta_{(d)} := \left\{y \in \mathbb{R}^d_+ : \sum_{i=1}^d y_i \le 1\right\} \quad \text{and} \quad I(p) := \{y \in \mathbb{R}^d : y_i = 0 \ (p_i = 0)\} \quad (p \in \mathbb{R}^d).$$

[5] Recall from the definition of $\mathcal{F}_P$ that $P_{\hat{\theta}}$ is the probability measure with $\frac{dP_{\hat{\theta}}}{dP}(y) = \exp(\langle y,\hat{\theta}\rangle - \psi_P(\hat{\theta}))$.

[6] One can evaluate Cramér's rate function value at a point of interest by solving a nonlinear system.

Reference Distribution (P)	Cramér Rate Function ($\psi_P^*(y)$)	$\operatorname{dom}\psi_P^*$
Multivariate Normal ($\mu \in \mathbb{R}^d, \Sigma \in \mathbb{S}^d : \Sigma \succ 0$)	$\frac{1}{2}(y-\mu)^T\Sigma^{-1}(y-\mu)$	$\mathbb{R}^d$
Multivar. Normal-inverse Gaussian $\big(\mu, \beta \in \mathbb{R}^d,\ \alpha, \delta \in \mathbb{R}, \Sigma \in \mathbb{R}^{d\times d}$: $\delta > 0,\ \Sigma \succ 0, \alpha \geq \sqrt{\beta^T\Sigma\beta}\big)$ $\gamma := \sqrt{\alpha^2 - \beta^T\Sigma\beta}$	$\alpha\sqrt{\delta^2 + (y-\mu)^T\Sigma^{-1}(y-\mu)} - \beta^T(y-\mu) - \delta\gamma$	$\mathbb{R}^d$
Gamma ($\alpha, \beta \in \mathbb{R}_{++}$)	$\beta y - \alpha + \alpha\log\left(\frac{\alpha}{\beta y}\right)$	$\mathbb{R}_{++}$
Laplace ($\mu \in \mathbb{R}, b \in \mathbb{R}_{++}$)	$\begin{cases} 0, & y = \mu, \\ \sqrt{1+\rho(y)^2} - 1 + \log\left(\frac{\sqrt{1+\rho(y)^2}-1}{\rho(y)^2/2}\right), & y \neq \mu, \end{cases}$ $(\rho(y) := (y-\mu)/b)$	$\mathbb{R}$
Poisson ($\lambda \in \mathbb{R}_{++}$)	$y\log(y/\lambda) - y + \lambda$	$\mathbb{R}_+$
Multinomial ($n \in \mathbb{N}, p \in \Delta_{(d)}$: $\sum_{i=1}^d p_i < 1$)	$\sum_{i=1}^d y_i \log\left(\frac{y_i}{np_i}\right) + \left(n - \sum_{i=1}^d y_i\right)\log\left(\frac{n-\sum_{i=1}^d y_i}{n(1-\sum_{i=1}^d p_i)}\right)$	$n\Delta_{(d)} \cap I(p)$
Negative Multinomial ($p \in [0,1)^d$, $y_0 \in \mathbb{R}_{++},\ p_0 := 1 - \sum_{i=1}^d p_i > 0$)	$\sum_{i=0}^d y_i \log\left(\frac{y_i}{p_i\bar{y}}\right)$ $\quad (\bar{y} := \sum_{i=0}^d y_i)$	$\mathbb{R}_+^d \cap I(p)$
Discrete Uniform $\big(a, b \in \mathbb{Z} : a \leq b$, $\mu := (a+b)/2, n := b-a+1\big)$	$\begin{cases} 0, & y = \mu, \\ (y-\mu)\theta - \log\left(\frac{e^{(b-\mu+1)\theta} - e^{(a-\mu)\theta}}{n(e^\theta - 1)}\right), & y \neq \mu, \end{cases}$ where $\theta \in \mathbb{R} :\ y + \frac{e^\theta}{e^\theta - 1} = \frac{(b+1)e^{(b+1)\theta} - ae^{a\theta}}{e^{(b+1)\theta} - e^{a\theta}}$	$[a, b]$
Continuous Uniform $\big(a, b \in \mathbb{R} : a < b, \mu := (a+b)/2\big)$	$\begin{cases} 0, & y = \mu, \\ (y-\mu)\theta - \log\left(\frac{e^{(b-\mu)\theta} - e^{(a-\mu)\theta}}{(b-a)\theta}\right), & y \neq \mu, \end{cases}$ where $\theta \in \mathbb{R} :\ y + \frac{1}{\theta} = \frac{be^{b\theta} - ae^{a\theta}}{e^{b\theta} - e^{a\theta}}$	(a, b)
Logistic ($\mu \in \mathbb{R}, s \in \mathbb{R}_{++}$)	$\begin{cases} 0, & y = \mu, \\ (y-\mu)\theta - \log\left(B(1-s\theta, 1+s\theta)\right), & y \neq \mu, \end{cases}$ where $\theta \in \mathbb{R}_+ :\ y - \mu = \frac{1}{\theta} + \frac{\pi s}{\tan(-\pi s\theta)}$	$\mathbb{R}$

Table 1: Cramér rate functions for popular distributions.

Remark 3.13 (On Table 1). We provide some additional comments on Table 1 here.

(a) (Special cases)
   - As special cases of the Gamma distribution we obtain Chi-squared with parameter k ($\alpha = k/2$, $\beta = 1/2$), Erlang (α positive integer) and exponential ($\alpha = 1$) distributions.

- As special cases of the multinomial distribution, we obtain binomial ($d = 1$, $n > 1$), Bernoulli ($d = 1$, $n = 1$) and categorical ($d > 1$, $n = 1$) distributions.
- As special cases of the negative multinomial distribution we obtain the negative binomial ($d = 1$) and (shifted) geometric ($d = 1$, $y_0 = 1$) distributions.

(b) (Statistical interpretation) For many reference distributions, ψ_P^* recovers well-known functions from information theory and related areas. Here, the MEM provides an information driven, statistical interpretation for these functions. Examples include the squared Mahalanobis distance (multivariate normal), pseudo-Huber loss (multivariate normal-inverse Gaussian), Itakura-Saito distance (Gamma), Burg entropy (exponential), Fermi-Dirac entropy (Bernoulli), and the generalized cross entropy (Poisson). $\diamondsuit$

4. The MEM Estimator and Models for Inverse Problems.

In this section we show how the MEM function can be used in various modeling paradigms. We start by presenting the MEM estimator and explore some of its properties. We then discuss its (primal and dual) analogy to the maximum likelihood (ML) estimator. Finally we will illustrate its efficacy by considering a class of linear models involving a regularization term.

4.1. The Maximum Entropy on the Mean Estimator.

The maximum entropy on the mean (MEM) function gives rise to an information driven criterion for measuring the compliance of given data with a prior distribution. Based on this function, we can define the MEM estimator as given in Definition 4.1 below. First, we introduce some additional terminology and notation that will be used in the sequel. Let $\Omega \subseteq \mathbb{R}^d$ and let $F_\Lambda = \{P_\lambda : \lambda \in \Lambda \subseteq \mathbb{R}^d\} \subset \mathcal{P}(\Omega)$ be a parameterized family of distributions indexed by $\lambda \in \Lambda$ such that $\mathbb{E}_{P_{\lambda_1}} = \mathbb{E}_{P_{\lambda_2}}$ if and only if $\lambda_1 = \lambda_2$. We call F_Λ as the *reference family* and say that it satisfies Assumptions 3.1 and 3.9 if they hold for each $P_\lambda \in F_\Lambda$. When F_Λ is an exponential family (in this case Λ is the natural parameter space Θ_P for some $P \in \mathcal{M}(\Omega)$) the MEM estimator was studied in [18, Chapter 6]. We stress that, in our presentation, F_Λ need *not* be an exponential family.

Definition 4.1 (MEM estimator). *Let $F_\Lambda \subset \mathcal{P}(\Omega)$ be a reference family satisfying Assumptions 3.1 and 3.9 and assume that $\mathbb{E}_{P_{\lambda_1}} = \mathbb{E}_{P_{\lambda_2}}$ if and only if $\lambda_1 = \lambda_2$. For an observation $\hat{y} \in \mathbb{R}^d$, let $P_{\hat{\lambda}} \in F_\Lambda$ be such that $\hat{y} = \mathbb{E}_{P_{\hat{\lambda}}}$, and let $S^* \subseteq \mathbb{R}^d$ be (nonempty) closed. The MEM estimator is defined as*

$$y_{MEM}(\hat{y}, F_\Lambda, S^*) := \operatorname{argmin}\{\psi^*_{P_{\hat{\lambda}}}(y) : y \in S^*\}.$$

In order to simplify notation, in what follows, we will write $y_{MEM} := y_{MEM}(\hat{y}, F_\Lambda, S^*)$ when the dependence on the triple $(\hat{y}, F_\Lambda, S^*)$ is clear from the context.

Remark 4.2 (The observation vector and its domain). In Definition 4.1, the condition that $P_{\hat{\lambda}} \in F_\Lambda$ is chosen such that $\hat{y} = \mathbb{E}_{P_{\hat{\lambda}}}$ implies that the reference distribution is indexed by the observation vector $\hat{y}$. This condition combined with Assumption 3.1 entails that $\hat{y} \in \operatorname{int} \Omega^{cc}_{P_{\hat{\lambda}}}$ must hold due to Lemma 3.4. $\diamondsuit$

In order to establish the well-definedness of the MEM estimator, we will use the following extension of [18, Lemma 5.4]. The proof is included in Appendix A.

Lemma 4.3. *Let* $\phi : \mathbb{R}^d \to (-\infty, +\infty]$ *be closed and Legendre-type, let* $\varphi : \mathbb{R}^d \to (-\infty, +\infty]$ *be proper, closed and convex such that* $\operatorname{int}(\operatorname{dom}\phi) \cap \operatorname{dom}\varphi \neq \emptyset$*. Assume that one of the functions is coercive while the other is bounded from below. Then there exists a unique solution* $y^* \in \mathbb{R}^d$ *to* $\min\{\phi(y) + \varphi(y) : y \in \mathbb{R}^d\}$*, which also satisfies* $y^* \in \operatorname{int}(\operatorname{dom}\phi) \cap \operatorname{dom}\varphi$*.*

Theorem 4.4 (Well-definedness of the MEM estimator). *Let* $F_\Lambda \subset \mathcal{P}(\Omega)$ *be a reference family satisfying Assumptions 3.1 and 3.9. For* $\hat{y} \in \mathbb{R}^d$*, let* $P_{\hat{\lambda}} \in F_\Lambda$ *such that* $\hat{y} = E_{P_{\hat{\lambda}}}$*, and let* $S^* \subseteq \mathbb{R}^d$ *be closed with* $S^* \cap \operatorname{dom}\psi^*_{P_{\hat{\lambda}}} \neq \emptyset$*. Then, the MEM estimator* y_{MEM} *exists. If, in addition,* S^* *is convex and* $\operatorname{int}(\operatorname{dom}\psi^*_{P_{\hat{\lambda}}}) \cap S^* \neq \emptyset$*,* y_{MEM} *is unique and in* $\operatorname{int}(\operatorname{dom}\psi^*_{P_{\hat{\lambda}}}) \cap S^*$*.*

Proof. Recall that, by Theorem 3.10, $\psi^*_{P_{\hat{\lambda}}}$ is coercive and of Legendre type (proper, closed, steep and strictly convex on the interior of its domain). Observe that $S^* \subset \mathbb{R}^d$ is closed and $S^* \cap \operatorname{dom}\psi^*_{P_{\hat{\lambda}}} \neq \emptyset$. Thus, the function $\psi^*_{P_{\hat{\lambda}}} + \delta_{S^*}$ is proper, closed and coercive. Hence, the existence of the MEM estimator follows from [2, Remark 3.4.1, Theorem 3.4.1]. The case when S^* is convex and $\operatorname{int}(\operatorname{dom}\psi^*_{P_{\hat{\lambda}}}) \cap S^* \neq \emptyset$ follows from Lemma 4.3 with $\phi = \psi^*_{P_{\hat{\lambda}}}$ and $\varphi = \delta_S$ due to the coercivity of $\psi^*_{P_{\hat{\lambda}}}$ and the fact that δ_S is bounded from below. ∎

4.1.1. Analogy Between MEM and ML (for Exponential Families).

Maximum likelihood (ML) is arguably the most popular principle for statistical estimation. Here, the estimated parameters are chosen as the most likely to produce a given sample of observed data while satisfying model assumptions. More precisely, for some $\Omega \subseteq \mathbb{R}^d$, the model is defined by means of a nonempty, closed set $S \subseteq \mathbb{R}^d$ of admissible parameters and a parameterized family of distributions $F_\Lambda = \{P_\lambda : \lambda \in \Lambda \subseteq \mathbb{R}^m\} \subset \mathcal{P}(\Omega)$ with densities f_{P_λ}. Given a sample of observed data $\hat{y} \in \mathbb{R}^d$, the ML estimator $\lambda_{ML}(\hat{y}, F_\Lambda, S)$ is defined as

$$\lambda_{ML}(\hat{y}, F_\Lambda, S) := \operatorname{argmax}\{\log f_{P_\lambda}(\hat{y}) : \lambda \in S \cap \Lambda\}.$$

In order to simplify notation, we will write $\lambda_{ML} := \lambda_{ML}(\hat{y}, F_\Lambda, S)$ when the dependence on the triple $(\hat{y}, F_\Lambda, S)$ is clear from the context.

An intriguing connection between the ML and MEM estimator comes to light when Λ is the natural parameter space Θ_P of an exponential family induced by $P \in \mathcal{M}(\Omega)$. The MEM estimator can then be retrieved by solving one of two alternative optimization problems each of which has a closely related problem that yields the ML estimator. One problem is driven by information theoretic arguments, while the other emphasizes a connection motivated by convex duality. These connections were previously observed in [18, Chapter 6] (also [14]) and are summarized in the following theorem whose proof is in Appendix A. For consistency, we denote the ML estimator as θ_{ML}.

Theorem 4.5 (MEM and ML estimator analogy). *Let* $\mathcal{F}_P$ *be a minimal and steep exponential family generated by* $P \in \mathcal{M}(\Omega)$ *and assume that, for any* $\theta \in \operatorname{int}\Theta_P$*, Assumption 3.9 holds with respect to* $P_\theta \in \mathcal{P}(\Omega)$*. Let* $S, S^* \subseteq \mathbb{R}^d$ *such that* $S \cap \operatorname{dom}\psi_P \neq \emptyset$ *and* $S^* \cap \operatorname{dom}\psi^*_P \neq \emptyset$*. Finally, let* $\hat{y} \in \operatorname{int}\Omega_P^{cc}$ *and set* $\hat{\theta} := \nabla\psi^*_P(\hat{y})$*. Then the following hold:*

(a) *(Primal analogy) If* $S^* \cap \operatorname{int}(\operatorname{dom}\psi^*_P) \neq \emptyset$ *and* $\nabla\psi^*_P(S^* \cap \operatorname{int}(\operatorname{dom}\psi^*_P)) = S \cap \operatorname{int}(\operatorname{dom}\psi_P)$*, then* $y_{MEM} = \nabla\psi_P(\theta_{MEM})$ *where*

$$\theta_{MEM} \in \operatorname{argmin}\{KL(P_\theta|P_{\hat{\theta}}) : \theta \in S\} \quad \textit{and} \quad \theta_{ML} \in \operatorname{argmin}\{KL(P_{\hat{\theta}}|P_\theta) : \theta \in S\}. \tag{4.1}$$

(b) (Dual analogy): We have

$$y_{MEM} \in \operatorname{argmin}\{D_{\psi_P^*}(y, \hat{y}) : y \in S^*\} \quad \textit{and} \quad \theta_{ML} \in \operatorname{argmin}\{D_{\psi_P}(\theta, \hat{\theta}) : \theta \in S\}. \tag{4.2}$$

The primal and dual analogy between the MEM and ML estimator for exponential families clarifies that the two are symmetric principles.

4.2. Examples - Linear Models. To illustrate the versatility of the MEM estimation framework, we will consider the broad class of linear models which are among the most popular paradigms in statistical estimation with applications in numerous fields such as image processing, bio-informatics, machine learning etc.

We assume that the set S^* of admissible mean value parameters is the image of a convex set $X \subseteq \mathbb{R}^d$ under a linear mapping defined by a measurement matrix $A \in \mathbb{R}^{m \times d}$. In many practical scenarios, this matrix satisfies some application-related properties, which in combination with the set X restricts the image space to a subset of $\mathbb{R}^m$. We will denote by $\mathcal{C}$ the set of all matrices that satisfy such a condition for the application in question. The second component in the model is $F_\Lambda = \{P_\lambda : \lambda \in \Lambda \subseteq \mathbb{R}^m\} \subset \mathcal{P}(\Omega)$, a reference family indexed by $\lambda \in \Lambda$ such that $\mathbb{E}_{P_{\lambda_1}} = \mathbb{E}_{P_{\lambda_2}}$ if and only if $\lambda_1 = \lambda_2$. The reference distribution is specified from this family by means of the observation vector $\hat{y}$. From Remark 4.2 it follows that such a family of distributions must satisfy $\hat{y} \in \operatorname{int} \Omega^{cc}_{P_{\hat{\lambda}}}$ for $\hat{\lambda}$ such that $\mathbb{E}_{P_{\hat{\lambda}}} = \hat{y}$. In some cases, this condition imposes additional assumptions that must be satisfied by the measurement vector. We will denote the set of measurement vectors that satisfy such an assumption with respect to the family of distributions under consideration by $D := \{y \in \mathbb{R}^m : \mathbb{E}_{P_\lambda} = y \ (\lambda \in \Lambda)\}$. To summarize, an MEM estimator of the linear model outlined above is obtained by solving

$$\min\left\{\psi^*_{P_{\hat{\lambda}}}(Ax) : x \in X\right\} \qquad (\hat{\lambda} \in \Lambda : \mathbb{E}_{P_{\hat{\lambda}}} = \hat{y}), \tag{4.3}$$

under the following set of assumptions:

Assumption 4.6 (MEM estimation for linear models).

1. *The reference family F_Λ satisfies Assumptions 3.1 and 3.9.*
2. *The set $X \subseteq \mathbb{R}^d$ is nonempty and convex.*
3. *$A \in \mathcal{C}$ and for any $x \in X$ it holds that $Ax \in \operatorname{dom} \psi_P^*$.*
4. *The observation vector satisfies $\hat{y} \in D$.*

In the following table, we present some examples of MEM linear models that correspond to particular choices of a reference family. In all cases, we assume that the reference family admits a separable structure as outlined in Remark 3.12. The vectors a_i $(i = 1, \ldots, m)$ stand for the ith row of the matrix A. We set

$$\mathcal{C}_0 := \{A \in \mathbb{R}_+^{m \times d} : \text{A has no zero rows or columns}\}.$$

Reference family	Objective function ($\psi^*_{P_{\hat{\lambda}}} \circ A$)	$\mathcal{C}$	X	D
Normal	$\frac{1}{2}\|Ax - \hat{y}\|_2^2$	$\mathbb{R}^{m\times d}$	$\mathbb{R}^d$	$\mathbb{R}^m$
Poisson	$\sum_{i=1}^m [\langle a_i, x\rangle \log(\langle a_i, x\rangle/\hat{y}_i) - \langle a_i, x\rangle + \hat{y}_i]$	$\mathcal{C}_0$	$\mathbb{R}^d_+$	$\mathbb{R}^m_{++}$
Gamma ($\beta = 1$)	$\sum_{i=1}^m [\langle a_i, x\rangle - \hat{y}_i \log(\langle a_i, x\rangle) - (\hat{y}_i - \hat{y}_i \log(\hat{y}_i))]$	$\mathcal{C}_0$	$\mathbb{R}^d_{++}$	$\mathbb{R}^m_+$

Table 2: Linear models under the MEM estimation framework for various reference families.

Remark 4.7. Additional models are readily available by choosing any of the reference distributions presented in Table 1. Alternatively, one may consider a family of linear models where the natural parameters are the ones restricted to the image of a convex set under a linear mapping. This class of models is commonly referred to as *generalized linear models* with a *canonical link function* [44]. ◊

The MEM linear model with reference family that corresponds to the normal distribution coincides with its ML counterpart, resulting in the celebrated least-squares model [15]. This phenomenon is unique for the normal distribution and is a direct consequence of the fact that the squared Euclidean norm is the only self-conjugate function [48, Section 12].

Linear inverse models under the Poisson noise assumption have been successfully applied in various disciplines including fluorescence microscopy, optical/infrared astronomy and medical applications such as positron emission tomography (PET) (see, for example, [14, 53]). The MEM linear model with Poisson reference distribution outlined in Table 2 was previously suggested in [6, Subsection 5.3] as an example for the algorithmic setting considered in that work (see further details in Section 5 where we expand on the framework considered in [6]).

If, for example, $X = \mathbb{R}^d$ and $\mathrm{rge}A = \mathbb{R}^m$ with $m < d$, then $x \in \mathbb{R}^d$ such that $y_{ML} = y_{MEM} = Ax = \hat{y}$. This outcome is not a result of a deep statistical characteristic but a simple consequence of the model's ill-posedness, a situation when the desired solution is not uniquely characterized by the model. Situations like this are among the reasons which motivate the use of *regularizers* which allow to incorporate some additional (prior) knowledge of the solution. This approach give rise to the following extended version of model (4.3)

$$\text{(4.4)} \qquad \min\left\{\psi^*_{P_{\hat{\lambda}}}(Ax) + \varphi(x) : x \in X\right\} \qquad (\hat{\lambda} \in \Lambda : \mathbb{E}_{P_{\hat{\lambda}}} = \hat{y}),$$

where, in our setting, $\varphi : \mathbb{R}^d \to (-\infty, +\infty]$ stands for a proper, closed and convex function. In (4.4), the optimization formulation is designed to find a solution (model estimator) that balances between two criteria represented by the *fidelity* term $\psi^*_{P_{\hat{\lambda}}} \circ A$ and the *regularization* term φ. While the fidelity term penalizes the violation between the model and observations, the regularization term incorporates prior information (belief) on the solution, and in many cases, when the problem with the fidelity term alone is ill-posed, it also serves as a regularizer.

In the context of MEM, the Cramér rate function can be used to penalize violations of the solution vector $x \in \mathbb{R}^d$ with respect to some prior reference measure $R \in \mathcal{P}(\Omega)$ that satisfies Assumptions 3.1 and 3.9. In other words, we can set $\varphi(x) = \psi_R^*(x)$.

In many applications, the desired reference distribution of the regularizer will admit a separable structure (à la Remark 3.12). While this is advantageous from an algorithmic perspective (cf. Remark 5.3), other alternatives are viable. Non-separable priors can be considered in order to promote desirable correlations between the entries of the solution to problem (4.4). E.g., by considering the multinomial, negative multinomial, multivariate normal inverse Gaussian or multivariate normal (with non-diagonal correlation matrix in the latter) reference distributions intrinsically give rise to non-separable modeling. But there are other options which involve separable reference distributions with a composite structure such as

$$\varphi(x) = \psi_R^*(Lx) \qquad \text{or} \qquad \varphi(x) = \sum_{i=1}^{d} \psi_R^*(L_i x), \tag{4.5}$$

where $L \in \mathbb{R}^{r \times d}, L_i \in \mathbb{R}^{r \times d}$. For example, new variants of the well-known (discrete) *total variation* (TV) regularizer [51] can be considered by replacing the norm appearing in the original definition by a Cramér rate function while keeping the first-order finite difference matrix (further details are given in the end of Section 5). Different reference distributions might be used to promote desirable, application-specific, properties of the solution. Nevertheless, for all choices of reference distribution the resulting function will admit some desirable properties, including convexity, differentiability and coerciveness as established in Theorem 3.10. As we will see in the following section, these properties allows us to consider a unified algorithmic approach for tackling problem (4.4).

5. Algorithms.

The optimization formulations of statistical estimation problems as presented in the previous section are solved by optimization algorithms. Customized methods, such as the ones we consider here, allow to leverage the structure of a given problem, thus resulting in a significant efficiency improvement compared to general purpose solvers. The structure of problems which are of interest for us is given by the *additive composite model*

$$\min\{f(x) + g(x) : x \in \mathbb{R}^d\}, \tag{5.1}$$

where $f, g : \mathbb{R}^d \to (-\infty, +\infty]$ are proper, closed and convex.

We will assume that both the fidelity and regularization term, represented by f and g, respectively, are continuously differentiable on the interior of their domain. This assumption holds for all the modeling paradigms discussed in the previous section. In particular, model (4.4) is recovered with $f = \psi_P^* \circ A$ and $g = \psi_R^*$. Our focus on this type of problem is for convenience only as our goal is merely to illustrate how modern first-order methods can be used for computing MEM estimators, much like their popular ML counterparts. We point out that we are not limited to this setting. Other models can be considered as well, e.g., by blending a fidelity term originating from an MEM modeling paradigm with a traditional regularizer or vice versa. In this case, similar algorithms are applicable under suitable adjustments.

The method we consider is the *Bregman proximal gradient* (BPG) method. This first-order iterative algorithm admits a comparably mild per-iteration complexity and as such it is particularly suitable for contemporary large-scale applications. It is important to notice that many other methods, including second-order and primal-dual decomposition methods, can be also considered in some scenarios and can benefit from the operators derived in this work. Before we present the BPG method, we need to define its fundamental components [6, 16].

Smooth adaptable kernel: Let $f : \mathbb{R}^d \to (-\infty, +\infty]$ be proper, closed and continuously differentiable on $\mathrm{int}\,(\mathrm{dom}\, f)$. Then $h : \mathbb{R}^d \to (-\infty, +\infty]$ of Legendre type is a *smooth adaptable kernel* with respect to f if $\mathrm{dom}\, h \subseteq \mathrm{dom}\, f$ and there exists $L > 0$ such that $Lh - f$ is convex.

Bregman proximal operator: Let $g : \mathbb{R}^d \to (-\infty, +\infty]$ be closed and proper and $h : \mathbb{R}^d \to (-\infty, +\infty]$ of Legendre type. Then the *Bregman proximal operator* is defined as

$$\mathrm{prox}^h_g(\bar{x}) := \mathrm{argmin}\,\{g(x) + D_h(x, \bar{x}) : x \in \mathbb{R}^n\} \qquad (\bar{x} \in \mathrm{int}\,(\mathrm{dom}\, h)). \tag{5.2}$$

The BPG method is applicable under the following assumption.

Assumption 5.1. *Consider problem (5.1) and assume that there exists a function of Legendre type $h : \mathbb{R}^d \to (-\infty, +\infty]$ such that:*

1. *h is a smooth adaptable kernel with respect to f.*
2. *h induces a computationally efficient Bregman proximal operator with respect to g.*

The BPG method reads:

(BPG Method) Pick $t \in (0, 1/L]$ and $x^0 \in \mathrm{int}\,(\mathrm{dom}\, h)$. For $k = 0, 1, 2, \ldots$ compute

$$x^{k+1} = \mathrm{prox}^h_{tg}\left(\nabla h^*\left(\nabla h(x^k) - t\nabla f(x^k)\right)\right).$$

For $h = (1/2)\|\cdot\|_2^2$ and f convex, $Lh - f$ is convex if and only if ∇f is L-Lipschitz. In this case, the Bregman proximal operator reduces to the classical proximal operator and the BPG method is the well-knows proximal gradient algorithm [11].

The BPG method for solving (5.1) exhibits a sublinear convergence rate [6]. Under suitable assumptions, the convergence improves to linear [5]. Accelerated variants, which improve practical performance and have superior theoretical guarantees under additional assumptions, are also available [3, 12]. For simplicity's sake, we confine ourselves with the basic BPG scheme, but the operators to be presented can be readily applied to the enhanced algorithms.

In order to customize the method to a particular instance of problem (5.1), a smooth adaptable kernel and corresponding Bregman proximal operator must be specified. To illustrate this idea for MEM estimation, we focus on the linear models discussed in the previous section. In particular, we consider the model (4.4) where $\varphi = \psi_R^*$. We assume that Assumption 4.6 holds and that the prior reference measure $R \in \mathcal{P}(\Omega)$ satisfies Assumptions 3.1 and 3.9. Furthermore, we assume that $\mathrm{dom}\, \psi_R \subseteq X$ which allows us to disregard the constraint $x \in X$. The latter assumption holds in many practical situations and we assume it here for simplicity. Otherwise, one can simply apply the BPG method with $g = \psi_R^* + \delta_X$ (under the appropriate adjustments to the proximal operator). In Table 3 below, we summarize the smooth adaptable kernels suitable for the models described in the previous section, see Table 2. In all cases, the smooth adaptable function admits a separable structure of the form $h(x) = \sum_{j=1}^d h_j(x_j)$ where $h_j : \mathbb{R} \to (-\infty, +\infty]$ $(j = 1, \ldots, d)$ is a (univariate) function of Legendre type. As we will see in what follows, this property is very desirable as it give rise to a computationally efficient implementation of the Bregman proximal operator. For completeness, we include the explicit formulas for the operators involved in the BPG method.

Reference family	Kernel (h_j)	Constant (L)	$[\nabla h(x)]_j$	$[\nabla h^*(z)]_j$
Normal	$(1/2)x_j^2$	$\|A\|_2 := \sqrt{\lambda_{\max}(A^TA)}$	x_j	z_j
Poisson	$x_j \log(x_j)$	$\|A\|_1 := \max_{j=1,2,\dots,d} \sum_{i=1}^m \|A_{i,j}\|$	$\log(x_j)+1$	$\exp(z_j-1)$
Gamma ($\beta=1$)	$-\log(x_j)$	$\|\hat{y}\|_1 := \sum_{i=1}^m \|\hat{y}_i\|$	$-1/x_j$	$-1/z_j$

Table 3: Smooth adaptable kernels and related operators that correspond to the objective function ($f = \psi^*_{P_{\hat{\theta}}} \circ A$) of the linear models listed in Table 2.

The kernel and related constant that correspond to the normal reference family is a well-known consequence due to the Lipschitz gradient continuity, a special case of the smooth adaptability property considered here.[7] The kernel and related constant that correspond to the Poisson reference family is due to [6, Lemma 8]. The kernel and related constant that correspond to the Gamma distribution follows from [6, Lemma 7].

We now discuss the special form of the Bregman proximal operator in the setting of the linear model (4.4) with $\varphi = \psi^*_R$. According to (5.2), for any $t > 0$, the Bregman proximal operator is defined by the smooth adaptable kernel h and the regularizer $g = \psi^*_R$ as follows:

$$\operatorname{prox}^h_{t\psi^*_R}(\bar{x}) = \operatorname{argmin}\left\{ t\psi^*_R(u) + D_h(u,\bar{x}) : u \in \mathbb{R}^d \right\}. \tag{5.3}$$

The following theorem records that, in our setting, the above operator is well defined.

Theorem 5.2 (Well-definedness of the Bregman proximal operator). *Let $h : \mathbb{R}^d \to (-\infty, +\infty]$ be of Legendre type and let $R \in \mathcal{P}(\Omega)$ be a reference distribution satisfying the conditions in Assumptions 3.1 and 3.9. Assume further that $\operatorname{int}(\operatorname{dom} h) \cap \operatorname{dom} \psi^*_R \neq \emptyset$. Then, for any $t > 0$ and $\bar{x} \in \operatorname{int}(\operatorname{dom} h)$, the Bregman proximal operator defined in (5.3) produces a unique point in $\operatorname{int}(\operatorname{dom} h) \cap \operatorname{dom} \psi^*_R$.*

Proof. Since $\bar{x} \in \operatorname{int}(\operatorname{dom} h)$, the function $D_h(\cdot,\bar{x})$ is proper. In addition, since h is of Legendre type, so is $D_h(\cdot,\bar{x})$. Finally, $D_h(\cdot,\bar{x})$ is bounded below (by zero) by convexity of h. The result follows from Lemma 4.3 with $\phi = D_h$ and $\varphi = t\psi^*_R$ due to the aforementioned properties of D_h and the coercivity of $t\psi^*_R$ (Theorem 3.10 and $t > 0$). ∎

We now show that this operator is also computationally tractable. For many reference distributions, this fact stems from the following separability property.

[7] More precisely, the equivalence holds for convex functions such as the ones considered here. For the nonconvex case see an extension of the smooth adaptability condition presented in [16].

Remark 5.3 (Separability of the Bregman proximal operator). In all cases under consideration, the smooth adaptable kernel $h : \mathbb{R}^d \to (-\infty, +\infty]$ admits a separable structure $h(x) = \sum_{j=1}^d h_j(x_j)$. Therefore, by (2.4), the induced Bregman distance satisfies: $D_h(x,y) = \sum_{i=1}^d D_{h_i}(x_i, y_i)$. If, in addition, the Cramér rate function admits a separable structure $\psi_R^* = \sum_{i=1}^d \psi_{R_i}^*$ (cf. Remark 3.12), then the optimization problem defining the Bregman proximal operator is separable and can be evaluated for each component of $\bar{x}$. $\diamondsuit$

Given a particular instance of problem (5.1), with fidelity term $f = \psi_{P_{\hat{\lambda}}}^* \circ A$ and regularizer $g = \psi_R^*$, one can derive a formula for the corresponding Bregman proximal operator. These formulas are summarized in Tables 4, 5, and 6 for each of the combinations of linear models (by using a compatible kernel generating distance from Table 3) and regularizers from Table 1. Some formulas are given in a closed form, others must be evaluated numerically through a solution of a nonlinear system.[8] Due to Remark 5.3, for most of the regularizer reference distributions (excluding only the multivariate normal, multinomial and negative multinomial) the resulting subproblem is separable. Thus, for the sake of simplicity and without loss of generality, we assume that $d = 1$, i.e., the resulting formulas correspond to one entry of the vector produced by the operator. The general case follows by applying the operator components-wise on all the elements of a vector $\bar{x} \in \mathbb{R}^d$. An implementation of the operators along with selected algorithms, applications, and detailed derivations of the operators can be found under:

https://github.com/yakov-vaisbourd/MEMshared.

The following table lists the formulas of Bregman proximal operators for the normal linear family. In this case, the operator reduces to the classical proximal operator [41].

Reference Distribution (R)	Proximal Operator ($x^+ = \mathrm{prox}_{t\psi_R^*}(\bar{x})$)
Multivariate Normal ($\mu \in \mathbb{R}^d, \Sigma \in \mathbb{S}^d : \Sigma \succ 0$)	$x^+ = (tI + \Sigma)^{-1}(\Sigma\bar{x} + t\mu)$
Multivariate Normal-inverse Gaussian $\left(\mu, \beta \in \mathbb{R}^d,\ \alpha, \delta \in \mathbb{R},\ \Sigma \in \mathbb{R}^{d\times d} : \delta > 0,\ \Sigma \succ 0,\ \alpha^2 \geq \beta^T\Sigma\beta,\ \gamma := \sqrt{\alpha^2 - \beta^T\Sigma\beta}\right)$	$x^+ = \left(I + \rho\Sigma^{-1}\right)^{-1}\left(t\beta + \bar{x} + \rho\Sigma^{-1}\mu\right)$, where $\rho \in \mathbb{R}_+ :$ $(\rho\delta)^2 + \Vert \left(\rho^{-1}I + \Sigma^{-1}\right)^{-1}(t\beta + \bar{x} - \mu) \Vert_{\Sigma^{-1}}^2 = (\alpha t)^2$
Gamma ($\alpha, \beta \in \mathbb{R}_{++}$)	$x^+ = \left(\bar{x} - t\beta + \sqrt{(\bar{x} - t\beta)^2 + 4t\alpha}\right)/2$

continued ...

[8]The solution of the nonlinear system can be efficiently approximated by various methods. In our implementation, building upon the fact that the systems involve monotonic functions (since they stem from the optimality conditions of a convex problem), we used a variant of safeguarded Newton-Raphson method.

. . . continued

Reference Distribution (R)	Proximal Operator ($x^+ = \mathrm{prox}_{t\psi_R^*}(\bar{x})$)
Laplace ($\mu \in \mathbb{R},\ b \in \mathbb{R}_{++}$)	$x^+ = \begin{cases} \mu, & \bar{x} = \mu, \\ \mu + b\rho, & \bar{x} \neq \mu, \end{cases}$ where $\rho \in \mathbb{R}: \quad \alpha_1\rho^3 + \alpha_2\rho^2 + \alpha_3\rho + \alpha_4 = 0$, with $\alpha_1 = (b/t)^2 b^2,\ \alpha_2 = 2(b/t)^2 b(\mu - \bar{x})$, $\alpha_3 = (b/t)^2(\mu - \bar{x})^2 - 2(b/t)b - 1,\ \alpha_4 = -2(b/t)(\mu - \bar{x})$
Poisson[9] ($\lambda \in \mathbb{R}_{++}$)	$x^+ = tW\left(\frac{\lambda e^{\bar{x}/t}}{t}\right)$
Multinomial ($n \in \mathbb{N}, p \in \Delta_{(d)}$: $\sum_{i=1}^d p_i < 1$)	$x^+ \in \mathbb{R}_+^d \cap I(p): \quad (x_i^+ - \bar{x}_i)/t + \log\left(\frac{x_i^+(1-\sum_{j=1}^d p_j)}{p_i(n-\sum_{j=1}^d x_j^+)}\right) = 0$
Negative Multinomial ($p \in [0,1)^d$, $x_0 \in \mathbb{R}_{++},\ p_0 := 1 - \sum_{i=1}^d p_i > 0$)	$x^+ \in \mathbb{R}_+^d \cap I(p): \ (x_i^+ - \bar{x}_i)/t + \log\left(\frac{x_i^+}{p_i(x_0+\sum_{j=1}^d x_j^+)}\right) = 0,$
Discrete Uniform ($a, b \in \mathbb{R} : a < b$)	$x^+ = \bar{x} - t\theta^+$ where $\theta^+ = 0$ if $\bar{x} = (a+b)/2$, otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $t(\theta^+ - \bar{x}/t) + \frac{(b+1)e^{(b+1)\theta^+} - ae^{a\theta^+}}{e^{(b+1)\theta^+} - e^{a\theta^+}} = \frac{e^{\theta^+}}{e^{\theta^+}-1}$
Continuous Uniform ($a, b \in \mathbb{R} : a \leq b$)	$x^+ = \bar{x} - t\theta^+$ where $\theta^+ = 0$ if $\bar{x} = (a+b)/2$, otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $t(\theta^+ - \bar{x}/t) + \frac{be^{b\theta^+} - ae^{a\theta^+}}{e^{b\theta^+} - e^{a\theta^+}} = \frac{1}{\theta^+}$
Logistic ($\mu \in \mathbb{R},\ s \in \mathbb{R}_{++}$):	$x^+ = \bar{x} - t\theta^+$ where $\theta^+ = 0$ if $\bar{x} = \mu$, otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $t\theta^+ + \frac{1}{\theta^+} + \frac{\pi s}{\tan(-\pi s\theta^+)} = \bar{x} - \mu$

Table 4: Bregman Proximal Operators - Normal Linear Model ($h = \frac{1}{2}\|\cdot\|^2$).

Recall that the Cramér rate function induced by a uniform (discrete/continuous) or logistic reference distribution does not admit a closed form. To compute their proximal operator we appeal to the corresponding dual of the subproblem in (5.3). This is done via Moreau decomposition (see, e.g., [11, Theorem 6.45]) which applies when the Bregman proximal operator (5.3) reduces to the classical proximal operator (i.e., when $h = (1/2)\|\cdot\|_2^2$). For the

[9] We denote by $W : \mathbb{R} \to \mathbb{R}$ the Lambert W function (see, for example, [23]).

general case, we will employ a result summarized in Lemma 5.4 and Corollary 5.5 below. The proofs of both results can be found in Appendix A. Some notation is needed: for a function $g : \mathbb{R}^d \to (-\infty, +\infty]$ proper, closed and convex and of $h : \mathbb{R}^d \to (-\infty, +\infty]$ of Legendre type we set

$$\mathrm{iconv}_g^h(\bar{x}) := \operatorname{argmin}\left\{g(x) + h(\bar{x} - x) : x \in \mathbb{R}^d\right\}. \tag{5.4}$$

This is the (possibly empty) solution of the optimization problem defining the *infimal convolution* $(g\Box h)(\bar{x}) := \inf\left\{g(x) + h(\bar{x} - x) : x \in \mathbb{R}^d\right\}$.

Lemma 5.4. *Let $g : \mathbb{R}^d \to (-\infty, +\infty]$ be proper, closed and convex and let $h : \mathbb{R}^d \to (-\infty, +\infty]$ be of Legendre type. Let $\bar{x} \in \mathrm{int}\,(\mathrm{dom}\, h)$ and assume that there exists a unique point $x^+ := \mathrm{prox}_g^h(\bar{x})$ satisfying $x^+ \in \mathrm{int}\,(\mathrm{dom}\, h) \cap \mathrm{dom}\, g$. Then, $y^+ := \mathrm{iconv}_{g^*}^{h^*}(\nabla h(\bar{x}))$ exists and it holds that $\nabla h(x^+) + y^+ = \nabla h(\bar{x})$.*

The following corollary adapts the above lemma to the setting considered in our study. Furthermore, we complement this result with a simple observation which is particularly useful for Bregman proximal operator computations.

Corollary 5.5. *Let $h : \mathbb{R}^d \to (-\infty, +\infty]$ be of Legendre type and let $R \in \mathcal{P}(\Omega)$ satisfy Assumptions 3.1 and 3.9. Assume further that $\mathrm{int}\,(\mathrm{dom}\, h) \cap \mathrm{dom}\, \psi_R^* \neq \emptyset$. For $t > 0$ and $\bar{x} \in \mathrm{int}\,(\mathrm{dom}\, h)$, let $x^+ := \mathrm{prox}_{t\psi_R^*}^h(\bar{x})$ and $\theta^+ := \mathrm{iconv}_{t\psi_R(\cdot/t)}^{h^*}(\bar{x})$. Then, $\nabla h(x^+) + \theta^+ = \nabla h(\bar{x})$. In particular, $\theta^+ = 0$ (and $x^+ = \bar{x}$) if and only if $\bar{x} = \mathbb{E}_R$.*

The formulas of Bregman proximal operators for the Poisson and Gamma ($\beta = 1$) linear families are included in Appendix A. We close our study with particular models and algorithms.

Barcode Image Deblurring. Restoration of a blurred and noisy image represented by a vector $\hat{y} \in \mathbb{R}^d$ can be cast as the following optimization problem:

$$\min\left\{\frac{1}{2}\|Ax - \hat{y}\|_2^2 + \tau\varphi_R^*(x) : x \in \mathbb{R}^d\right\}. \tag{5.5}$$

$A \in \mathbb{R}^{d\times d}$ is the blurring operator and $\tau > 0$ is a regularization parameter. The noise is assumed to be Gaussian which explains the least-squares fidelity term which can be justified from the viewpoint of both the ML and, as we know from our study, the MEM framework. If the original image is a 2D barcode, a natural choice for the reference measure $R \in \mathcal{P}(\Omega)$ inducing φ_R^* is a separable Bernoulli distribution with $p = 1/2$ due to the binary nature of each pixel and no preference at each pixel to take either value.[10] Additional information (symbology) can be easily incorporated by an appropriate adjustment of the parameter for each known pixel (see [47]). Using the appropriate proximal operator from Table 4, the BPG method for solving the model takes the form

$$x_i^{k+1} \in \mathbb{R} : \quad x_i^{k+1} + t\tau \log\left(\frac{x_i^{k+1}}{1 - x_i^{k+1}}\right) = x_i^k - t[A^T(Ax^k - \hat{y})]_i, \quad (i = 1, 2, \dots, d).$$

[10] As mentioned in Remark 3.13, Bernoulli is a special case of the multinomial distribution. This, one dimensional, distribution is used to form a d-dimensional i.i.d as described in Remark 3.12.

As mentioned above, our focus on the Bregman proximal gradient method is only for illustration purposes. Favorable accelerated algorithms that employ the proximal operators derived in this work are readily available and should be used in practice. The acceleration scheme applicable here is known as the Fast Iterative Shrinkage Thresholding Algorithm (FISTA) [12].

Natural Image Deblurring. For natural image deblurring there is no obvious structure such as the binary one for barcodes. However, it is customary to assume that the image is piecewise smooth. A popular model that promotes piecewise constant restoration is the Rudin, Osher and Fatemi (ROF) model [51] based on the total variation (TV) regularizer $\sum_{i=1}^{d} g(L_i x)$. Here, $L_i \in \mathbb{R}^{2\times d}$ extracts the difference between the pixel i and two adjacent pixels while g stands for either the l_1 (isotropic TV) or l_2 (anisotropic TV) norm. Variants which admit the same structure with other choices of g are also considered in the literature: in [21, Subsection 6.2.3], a model with the Huber norm for g was shown to promote restoration prone to artificial flat areas. Alternatively, one may consider the pseudo-Huber norm that corresponds to an MEM regularizer induced by the multivariate normal inverse-Gaussian reference distribution with parameters $\mu = \beta = 0$, $\alpha = 1$ and $\Sigma = I$. The resulting model is similar to (5.5) where the regularization term is substituted by $\sum_{i=1}^{d} \psi_R^*(L_i x)$. This model can be tackled by a primal-dual decomposition method that employs the appropriate proximal operator from Table 4. For example, using the separability of the proximal operator [11, Theorem 6.6] and the extended Moreau decomposition [11, Theorem 6.45], the update formula of the Chambolle-Pock algorithm [21, Algorithm 1] reads

$$
\begin{aligned}
y_i^{k+1} &= \tfrac{\rho_i}{1+\rho_i}(y^k + sL_i z^k) \qquad\qquad (i = 1, 2, \ldots, d),\\
\text{with}\quad & \rho_i \in \mathbb{R}_+ : \rho_i^2 (s\delta)^2 + \left(\tfrac{\rho_i}{1+\rho_i}\right)^2 \|y_i^k + sL_i z^k\|_2^2 = 1,\\
x^{k+1} &= (I + \tau A^T A)^{-1}\left(x^k - \tau(L^T y^{k+1} - A^T \hat{y})\right),\\
z^{k+1} &= 2x^{k+1} - x^k,
\end{aligned}
$$

where $L^T = [L_1^T, \ldots, L_d^T] \in \mathbb{R}^{d\times 2d}$, $y^k \in \mathbb{R}^{2d} : (y^k)^T = [(y_1^k)^T, \ldots, (y_d^k)^T]$ with $y_i^k \in \mathbb{R}^2$ for all $i = 1, 2, \ldots, d$) and s, τ are some positive step-sizes satisfying $s\tau\|L\|_2^2 < 1$.

We point out that an efficient implementation of the above algorithm that takes into account the sparse and structured nature of the matrices L and A, respectively, will result in a per-iteration complexity of the order $O(d \log d)$. The same statement is true with regard to the BPG method in the previous and following examples.

Poisson Linear Inverse Problem. Poisson linear inverse problems play a prominent role in various physical and medical imaging applications. The linear model proposed in [6, Subsection 5.3] is simply the MEM linear model with Poisson reference distribution. The authors of [6] suggest l_1-regularization to deploy their BPG method. Alternatively, one may consider the MEM function induced by the Laplace distribution with parameters $\mu = 0$ and $b = 1$.

This setting leads to the following update formula of the BPG method. For $i = 1, 2, \dots, d$:

$$\begin{aligned} \bar{x}_i^{k+1} &= \exp\left(\log(x_i^k) - t\sum_{j=1}^{m} a_{ji}\log(\langle a_j, x^k\rangle/\hat{y}_j)\right), \\ x_i^{k+1} \in \mathbb{R}: \quad t^2 x_i^{k+1} + 2t\log\left(\frac{x_i^{k+1}}{\bar{x}_i^{k+1}}\right) &= x_i^{k+1}\left[\log\left(\frac{x_i^{k+1}}{\bar{x}_i^{k+1}}\right)\right]^2. \end{aligned}$$

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Appendix A. Deferred Proofs and Tables.

A.1. Deferred Proofs.

Proof (for Lemma 3.11). For $y \in \operatorname{dom} \psi_P^*$, we have

$$\begin{aligned}\psi^*_{P_{\hat\theta}}(y) &\overset{(3)}{=} \sup\left\{\langle y,\theta\rangle - \log\left(M_{P_{\hat\theta}}[\theta]\right) : \theta \in \mathbb{R}^d\right\}\\ &\overset{(3.9)}{=} \sup\left\{\langle y,\theta\rangle - [\psi_P(\hat\theta+\theta) - \psi_P(\hat\theta)] : \theta\in\mathbb{R}^d\right\}\\ &= \psi_P^*(y) + \psi_P(\hat\theta) - \langle y,\hat\theta\rangle.\end{aligned}$$

The result follows from the definition of the Bregman distance, (2.2) and $\hat\theta \in \operatorname{int}(\operatorname{dom}\psi_P)$. ∎

Proof (for Lemma 4.3). Existence and uniqueness of the solution follows from [9, Corollary 11.15]. It remains to show that $y^* \in \operatorname{int}(\operatorname{dom}\phi) \cap \operatorname{dom}\varphi$. Evidently, $y^* \in \operatorname{dom}\phi \cap \operatorname{dom}\varphi$ thus it is sufficient to show that $y^* \in \operatorname{int}(\operatorname{dom}\phi)$. Using [9, Theorem 16.2] and [9, Corollary 16.38] we have $0 \in \partial\phi(y^*) + \partial\varphi(y^*)$, in particular $\partial\phi(y^*) \neq \emptyset$. Since ϕ is of Legendre type we conclude that $y^* \in \operatorname{int}(\operatorname{dom}\phi)$ [48, Theorem 26.1]. ∎

Proof (for Theorem 4.5). Since $\mathcal{F}_P$ is assumed to be minimal and steep, it is easy to verify (recall (3.9)) that P_θ satisfies Assumption 3.1 for any $\theta \in \operatorname{int}\Theta_P$. As we assume $S \cap \operatorname{dom}\psi_P \neq \emptyset$ and $S^* \cap \operatorname{dom}\psi_P^* \neq \emptyset$, the MEM and ML estimator exist due to Theorem 4.4 and [18, Theorem 5.7], respectively. We now prove (b). Since $\mathcal{F}_P$ is an exponential family, we have $\log f_{P_\theta}(\hat y) = \langle \hat y,\theta\rangle - \psi_P(\theta)$ and the ML estimator is a solution to

$$\begin{aligned}\max\{\log f_{P_\theta}(\hat y) : \theta\in S\} &= \max\{\langle\hat y,\theta\rangle - \psi_P(\theta) : \theta \in S\}\\ &= -\min\{D_{\psi_P}(\theta, \nabla\psi_P^*(\hat y)) : \theta\in S\} - \psi_P(\nabla\psi_P^*(\hat y)) + \langle \hat y, \nabla\psi_P^*(\hat y)\rangle.\end{aligned}$$

Omitting terms independent of the minimization and using that $\hat\theta = \nabla\psi_P^*(\hat y)$, the formulation for the ML estimator follows. To obtain the formulation for the MEM estimator, observe that, due to Lemma 3.11, we have

$$\min\{\psi^*_{P_{\hat{\theta}}}(y) : y \in S^*\} = \min\{D_{\psi^*_P}(y, \nabla\psi_P(\hat{\theta})) : y \in S^*\}.$$

Thus, the result follows by recalling that $\hat{y} = \nabla\psi_P(\hat{\theta})$.

We now turn to prove (a). Since $S^* \cap \operatorname{int}(\operatorname{dom}\psi^*_P) \neq \emptyset$ we obtain by Theorem 4.4 that $y_{MEM} \in S^* \cap \operatorname{int}(\operatorname{dom}\psi^*_P)$. This fact combined with the assumption $\nabla\psi^*_P(S^* \cap \operatorname{int}(\operatorname{dom}\psi^*_P)) = S \cap \operatorname{int}(\operatorname{dom}\psi_P)$ implies that $\nabla\psi^*_P(y_{MEM}) \in S \cap \operatorname{int}(\operatorname{dom}\psi_P)$. Thus, (a) follows from (b) due to the Bregman distance dual representation property (2.3) and Remark 2.6. ■

Proof (for Lemma 5.4). By the optimality condition of the optimization problem in the definition of the Bregman proximal operator (5.2) we obtain that

$$\nabla h(\bar{x}) - \nabla h(x^+) \in \partial g(x^+).$$

Since g is assumed to be proper, closed and convex, (2.2) yields

$$x^+ \in \partial g^* \left(\nabla h(\bar{x}) - \nabla h(x^+)\right). \tag{A.1}$$

Setting $\tilde{y} := \nabla h(\bar{x}) - \nabla h(x^+)$ and observing that $x^+ = \nabla h^*(\nabla h(\bar{x}) - \tilde{y})$ we can rewrite (A.1) as

$$\nabla h^*(\nabla h(\bar{x}) - \tilde{y}) \in \partial g^*(\tilde{y}).$$

It is now easy to verify that the above is nothing else but the optimality condition for $\bar{y}$, thus, $\tilde{y} = y^+$ and we can conclude that $\nabla h(x^+) + y^+ = \nabla h(\bar{x})$, establishing the desired result. ■

Proof (for Corollary 5.5). By Theorem 3.10 we have that ψ^*_R is proper, closed and convex and thus $\psi^{**}_R = \psi_R$ due to [11, Theorem 4.8]. By Theorem 5.2 we know that x^+ is well defined. The proof of the first part then follows directly from Lemma 5.4 (with $g = t\psi^*_R$ and $y^+ = \theta^+$) and [11, Theorem 4.14(a)]. To see that $\theta^+ = 0$ if and only if $\bar{x} = \mathbb{E}_R$, observe that the objective function in the subproblem defining the Bregman proximal operator (5.3) is greater equal than zero, and equality holds if and only if $\bar{x} = \mathbb{E}_R$ with $x^+ = \bar{x}$. Thus, the statement holds true in view of the first part of the current corollary. ■

A.2. Bregman Proximal Operators for Poisson and Gamma ($\beta = 1$) Linear Families.

The following table lists the formulas of Bregman proximal operators for the Poisson and Gamma ($\beta = 1$) linear families, respectively. Observe that by Theorem 5.2 the Bregman proximal operator is well defined if $\operatorname{int}(\operatorname{dom} h) \cap \operatorname{dom}\psi^*_R \neq \emptyset$. Since $\operatorname{int}(\operatorname{dom} h) = \mathbb{R}^d_{++}$ this implies that for the multinomial and negative multinomial distributions we must assume that $p_i > 0$ for all $i = 1, 2, \ldots, d$. Furthermore, for the sake of simplicity we include the normal and normal inverse-Gaussian distributions. The multivariate variants can be found in the software documentation along with further explanations.

Reference Distribution (R)	Bregman Proximal Operator ($x^+ = \mathrm{prox}^h_{t\psi^*_R}(\bar{x})$)
Normal ($\mu, \sigma \in \mathbb{R}:\ \sigma > 0$)	$x^+ = \frac{\sigma}{t} W\left(\frac{t}{\sigma}\bar{x}e^{\frac{t\mu}{\sigma}}\right)$
Normal-inverse Gaussian $\big(\mu, \alpha, \beta, \delta \in \mathbb{R}:\ \delta > 0,\ \alpha \geq \lvert\beta\rvert,\ \gamma := \sqrt{\alpha^2 - \beta^2}\big)$	$x^+ \in \mathbb{R}_{++}:$ $(t\alpha/\sigma)(x^+ - \mu) = (t\beta - \log(x^+/\bar{x}))\sqrt{\delta^2 + (x^+ - \mu)^2/\sigma}$
Gamma ($\alpha, \beta \in \mathbb{R}_{++}$)	$x^+ = \frac{\alpha t}{W\left(\frac{\alpha t \exp(t\beta)}{\bar{x}}\right)}$
Laplace ($\mu \in \mathbb{R},\ b \in \mathbb{R}_{++}$)	$x^+ = \begin{cases} \mu, & \bar{x} = \mu, \\ \mu + b\rho, & \bar{x} \neq \mu, \end{cases}$ where $\rho \in \mathbb{R}:\quad \rho + \frac{2b}{t}\log\left(\frac{\mu + b\rho}{\bar{x}}\right) = \frac{b^2\rho}{t^2}\log^2\left(\frac{\mu + b\rho}{\bar{x}}\right)$
Poisson ($\lambda \in \mathbb{R}_{++}$)	$x^+ = \bar{x}^{1-\tau}\lambda^\tau \qquad (\tau := \frac{t}{t+1})$
Multinomial ($n \in \mathbb{N}, p \in \mathrm{int}\,\Delta_{(d)}$)	$x_i^+ = \gamma_i\,(n - \rho)^\tau \quad \left(\tau := \frac{t}{t+1},\ \gamma_i := \left[\frac{p_i \bar{x}_i{}^{1/t}}{1 - \sum_{j=1}^d p_j}\right]^\tau\right)$ where $\rho \in \mathbb{R}:\ \rho = (n - \rho)^{\frac{t}{t+1}}\left(\sum_{i=1}^d \gamma_i\right)$
Negative Multinomial ($p \in (0,1)^d$, $x_0 \in \mathbb{R}_{++},\ p_0 := 1 - \sum_{i=1}^d p_i > 0$)	$x^+ \in \mathbb{R}^d_+ \cap I(p):\ \log\left(\frac{x_i^+}{\bar{x}_i}\right) + t\log\left(\frac{x_i^+}{p_i(x_0 + \sum_{j=1}^d x_j^+)}\right) = 0,$
Discrete Uniform ($a, b \in \mathbb{R} : a < b$)	$x^+ = \bar{x}e^{-t\theta^+}$ where $\theta^+ = 0$ if $\bar{x} = (a+b)/2$, otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $\frac{(b+1)\exp((b+1)\theta^+) - a\exp(a\theta^+)}{\exp((b+1)\theta^+) - \exp(a\theta^+)} = \frac{\exp(\theta^+)}{\exp(\theta^+) - 1} + \exp(\bar{x} - t\theta^+ - 1)$
Continuous Uniform ($a, b \in \mathbb{R} : a \leq b$)	$x^+ = \bar{x}e^{-t\theta^+}$ where $\theta^+ = 0$ if $\bar{x} = (a+b)/2$, otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $\frac{b\exp(b\theta^+) - a\exp(a\theta^+)}{\exp(b\theta^+) - \exp(a\theta^+)} = \frac{1}{\theta^+} + \exp(\bar{x} - t\theta^+ - 1)$
Logistic ($\mu \in \mathbb{R},\ s \in \mathbb{R}_{++}$):	$x^+ = \bar{x}e^{-t\theta^+}$ where $\theta^+ = 0$ if $\bar{x} = \mu$, otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $\frac{1}{\theta^+} + \frac{\pi s}{\tan(-\pi s\theta^+)} + \mu = \exp(\bar{x} - t\theta^+ - 1)$

Table 5: Bregman Proximal Operators - Poisson Linear Model ($h_j(x) = x_j \log x_j$)

Reference Distribution (R)	Bregman Proximal Operator ($x^+ = \mathrm{prox}^h_{t\psi^*_R}(\bar{x})$)
Normal ($\mu, \sigma \in \mathbb{R}: \ \sigma > 0$)	$x^+ = \left((t/\sigma)\mu - 1/\bar{x} + \sqrt{((t/\sigma)\mu - 1/\bar{x})^2 + 4(t/\sigma)}\right)/(2t/\sigma)$
Normal-inverse Gaussian $\big(\mu, \alpha, \beta, \delta \in \mathbb{R}: \ \delta > 0,$ $\alpha \geq \lvert\beta\rvert, \ \gamma := \sqrt{\alpha^2 - \beta^2}\big)$	$x^+ \in \mathbb{R}_{++}:$ $t\alpha(x^+ - \mu)x^+ = \left((t\beta - 1/\bar{x})x^+ + 1\right)\sqrt{\delta^2 + (x^+ - \mu)^2}$
Multivariate Normal-inverse Gaussian $\big(\mu, \beta \in \mathbb{R}^d, \ \alpha, \delta \in \mathbb{R},$ $\Sigma = \sigma I, \sigma > 0 : \delta > 0, \ \Sigma \succ 0,$ $\alpha^2 \geq \beta^T\Sigma\beta, \gamma := \sqrt{\alpha^2 - \beta^T\Sigma\beta}\big)$	$x_i^+ = (w_i + \rho\mu_i + \sqrt{(w_i + \rho\mu_i)^2 + 4\rho})/(2\rho),$ with $w_i = t\beta_i - 1/\bar{x}_i$ and $\rho \in \mathbb{R}_+:$ $(\rho\delta)^2 + \frac{1}{4\sigma}\sum_{i=1}^d \left(w_i + \sqrt{(w_i + \mu_i\rho)^2 + 4\rho}\right)^2 = (\alpha t/\sigma)^2$
Gamma ($\alpha, \beta \in \mathbb{R}_{++}$)	$x^+ = \bar{x}(t\alpha + 1)/(\bar{x}t\beta + 1)$
Laplace ($\mu \in \mathbb{R}, \ b \in \mathbb{R}_{++}$)	$x^+ = \begin{cases} \mu, & \bar{x} = \mu, \\ \mu + b\rho, & \bar{x} \neq \mu, \end{cases}$ where $\rho \in \mathbb{R}: \quad \alpha_1\rho^3 + \alpha_2\rho^2 + \alpha_3\rho + \alpha_4 = 0,$ with $\alpha_1 = b^2((b/\bar{x})^2 - t^2), \ \alpha_2 = 2b(\mu((b/\bar{x})^2 - t^2) - b^2(t+1)/\bar{x}),$ $\alpha_3 = b^2((1 - \mu/\bar{x})^2 + 2t(1 - 2\mu/\bar{x})) - t^2\mu^2, \ \alpha_4 = 2tb\mu(1 - \mu/\bar{x})$
Poisson ($\lambda \in \mathbb{R}_{++}$)	$x^+ \in \mathbb{R}_+: \ t\log\left(\frac{x^+}{\lambda}\right) = \frac{1}{x^+} - \frac{1}{\bar{x}}$
Multinomial ($n \in \mathbb{N}, p \in \mathrm{ri}\,\Delta_{(d)}$)	$x^+ \in \mathrm{ri}\, n\Delta_{(d)}: \ t\log\left(\frac{x_i^+(1 - \sum_{j=1}^d p_j)}{p_i(n - \sum_{j=1}^d x_j^+)}\right) = \frac{1}{x_i^+} - \frac{1}{\bar{x}_i}$
Negative Multinomial ($p \in (0,1)^d$, $x_0 \in \mathbb{R}_{++}, \ p_0 := 1 - \sum_{i=1}^d p_i > 0$)	$x^+ \in \mathbb{R}^d_{++}: \ t\log\left(\frac{x_i^+}{p_i(x_0 + \sum_{i=j}^d x_j^+)}\right) = \frac{1}{x_i^+} - \frac{1}{\bar{x}_i},$
Discrete Uniform ($a, b \in \mathbb{R} : a < b$)	$x^+ = \bar{x}/(\bar{x}t\theta^+ + 1)$ where $\theta^+ = 0$ if $\bar{x} = (a+b)/2,$ otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $\frac{(b+1)\exp((b+1)\theta) - a\exp(a\theta)}{(\exp((b+1)\theta) - \exp(a\theta)} = \frac{\exp(\theta)}{\exp(\theta) - 1} + \frac{\bar{x}}{t\bar{x}\theta^+ + 1}$
Continuous Uniform ($a, b \in \mathbb{R} : a \leq b$)	$x^+ = \bar{x}/(\bar{x}t\theta^+ + 1)$ where $\theta^+ = 0$ if $\bar{x} = (a+b)/2,$ otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $\frac{b\exp(b\theta^+) - a\exp(a\theta^+)}{\exp(b\theta^+) - \exp(a\theta^+)} = \frac{1}{\theta^+} + \frac{\bar{x}}{t\bar{x}\theta^+ + 1}$
Logistic ($\mu \in \mathbb{R}, \ s \in \mathbb{R}_{++}$):	$x^+ = \bar{x}/(\bar{x}t\theta^+ + 1)$ where $\theta^+ = 0$ if $\bar{x} = \mu,$ otherwise: $\theta^+ \in \mathbb{R} \setminus \{0\}$: $\frac{1}{\theta^+} + \frac{\pi s}{\tan(-\pi s\theta^+)} + \mu = \frac{\bar{x}}{\bar{x}t\theta^+ + 1}$

Table 6: Bregman Proximal Operators - Gamma ($\beta = 1$) Linear Model ($h_j(x) = -\log(x_j)$)