

APPLICATIONS OF STRUCTURAL STATISTICS: GEOMETRICAL INFERENCE IN EXPONENTIAL FAMILIES

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ABSTRACT. Exponential families comprise a broad class of statistical models and parametric families like normal distributions, binomial distributions, gamma distributions or exponential distributions. Thereby the formal representation of its probability distributions induces a confined intrinsic structure, which appears to be that of a dually flat statistical manifold. Conversely it can be shown, that any dually flat statistical manifold, which is given by a regular Bregman divergence uniquely induced a regular exponential family, such that exponential families may with some restrictions be regarded as a universal representation of dually flat statistical manifolds. In this article the intrinsic structure of exponential families is derived.

1. PRIMARY AFFINE STRUCTURE OF EXPONENTIAL FAMILIES

Definition (Exponential family). *Let $(\Omega, \mathcal{F}_\theta)$ be a statistical model over a measurable space (Ω, Σ_Ω) . Then (Ω, \mathcal{F}) is termed an exponential family if and only if there exists an invertible function*

$$\xi : \text{dom}\theta \rightarrow \mathbb{R}^n$$

a sufficient statistic

$$T : (\Omega, \Sigma_\Omega) \rightarrow (\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$$

and a scalar function

$$f : \text{dom}\theta \rightarrow \mathbb{R}$$

such that for any $P_\theta \in \mathcal{F}$ and $\sigma \in \Sigma_\Omega$ it holds that:

$$(1.1) \quad P_\theta[\sigma] = \int_{\sigma} \exp(\xi(\theta_P) \cdot T(\omega)) d\mu(\omega) \cdot \int_{\sigma} \exp f(\theta_P) d\mu(\omega)$$

Since T is a sufficient statistic a Markov morphism, given by $\mathcal{T}(P)[\sigma] = P[T^{-1}(\sigma)]$ is globally invertible and its restriction to (Ω, \mathcal{F}) yields a statistical isomorphism $\mathfrak{T} \in \text{iso}(\mathbf{Stat})$ to a statistical model $(X, \mathcal{P}) := \text{img}\mathfrak{T}$ over a measurable space (X, Σ_X) . Then $\eta := \theta \circ \xi^{-1}$ is an identifiable parametrisation of (X, \mathcal{P}) and by the definition

$$\psi := \xi^{-1} \circ f \circ \xi$$

it follows that:

(1.2)

$$P_\eta[\sigma] = \int_{\sigma} \exp(\eta_P \cdot \mathbf{x} - \psi(\eta_P)) d\mathbf{x}, \forall \sigma \in \Sigma_X$$

Without loss of generality any exponential family, as defined in 1.1, may therefore be assumed to be given by probability distributions with a representation 1.2. This representation is termed the canonical form of an exponential family and the parametrisation η the canonical, or natural parametrisation.

Definition (Natural parametrisation). *Let $(X, \mathcal{P}) \in \text{ob}(\mathbf{Stat})$ be an exponential family in canonical form, then the corresponding canonical parametrisation η is termed a natural parametrisation of (X, \mathcal{P}) and the parameter vectors $\eta_P \in \text{dom}\eta \subseteq \mathbb{R}^n$ are termed natural parameters. **Remark:** Exponential families, given by the notation (X, \mathcal{P}_η) implicate a canonical form and a natural parametrisation η .*

The function $\psi : \mathbb{R}^n \rightarrow \mathbb{R}$, given by an exponential family in canonical form is known as the cumulant generating function and may be regarded as a normalisation factor, that implements the normalisation condition of the probability distribution:

$$(1.3) \quad \int_X \exp(\eta_P \cdot \mathbf{x} - \psi(\eta_P)) d\mathbf{x} = 1$$

Since $\psi(\boldsymbol{\eta}_P)$ is independent of \mathbf{x} it may be pulled out of the integral and a rearrangement of equation 1.3 yields:

$$(1.4) \quad \psi(\boldsymbol{\eta}_P) = \log \int_X \exp(\boldsymbol{\eta}_P \cdot \mathbf{x}) d\mathbf{x}$$

Due to this dependency the cumulant generating function relates different statistical properties.

Lemma 1. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) , then ψ is convex with respect to η and it's first and second order derivatives are given by:*

$$(1.5) \quad \nabla_\eta \psi(\boldsymbol{\eta}_P) = \mathbb{E}_\eta[\mathbf{x}]$$

$$(1.6) \quad \nabla_\eta^2 \psi(\boldsymbol{\eta}_P) = \text{Var}_\eta[\mathbf{x}]$$

where $\mathbb{E}_\eta[\mathbf{x}] \in \mathbb{R}^n$ and $\text{Var}_\eta[\mathbf{x}] \in \mathbb{R}^n$ respectively denote the vectorial expectation and variance of \mathbf{x} with respect to P_η .

Proof. Let $P_\eta \in \mathcal{P}$ and let p_η be the density function of P_η over (X, Σ_X) . Then the normalization condition is:

$$(1.7) \quad \int_X p_\eta(\mathbf{x}) d\mathbf{x} = 1$$

The partial derivation ∂_i of equation 1.7 to the natural parameter η_i yields:

$$\begin{aligned} & \partial_i \int_X p_\eta(\mathbf{x}) d\mathbf{x} \\ &= \int_X \partial_i \exp \left(\sum_{i=1}^n \eta_i x_i - \psi(\boldsymbol{\eta}_P) \right) d\mathbf{x} \\ (1.8) \quad &= \int_X (x_i - \partial_i \psi(\boldsymbol{\eta}_P)) p_\eta(\mathbf{x}) d\mathbf{x} \stackrel{1.7}{=} 0 \end{aligned}$$

Therefore:

$$\begin{aligned} & \nabla_\eta \psi(\boldsymbol{\eta}_P) \\ & \stackrel{1.7}{=} \nabla_\eta \psi(\boldsymbol{\eta}_P) \int_X p_\eta(\mathbf{x}) d\mathbf{x} \\ &= \int_X \nabla_\eta \psi(\boldsymbol{\eta}_P) p_\eta(\mathbf{x}) d\mathbf{x} \\ & \stackrel{1.8}{=} \int_X \mathbf{x} p_\eta(\mathbf{x}) d\mathbf{x} \\ &= \mathbb{E}_\eta[\mathbf{x}] \end{aligned}$$

This proves equation 1.5. A further partial derivation of 1.8 with respect to the natural parameter η_j yields:

$$\begin{aligned} 0 & \stackrel{1.8}{=} \partial_j \int_X (x_i - \partial_i \psi(\boldsymbol{\eta}_P)) p_\eta(\mathbf{x}) d\mathbf{x} \\ &= \int_X (x_i - \partial_i \psi(\boldsymbol{\eta}_P)) \partial_j p_\eta(\mathbf{x}) d\mathbf{x} \\ & \quad - \int_X \partial_j \partial_i \psi(\boldsymbol{\eta}_P) \int_X p_\eta(\mathbf{x}) d\mathbf{x} \\ (1.9) \quad & \stackrel{1.8}{=} \int_X (x_i - \partial_i \psi(\boldsymbol{\eta}_P)) (x_j - \partial_j \psi(\boldsymbol{\eta})) p_\eta(\mathbf{x}) d\mathbf{x} \\ & \quad - \partial_j \partial_i \psi(\boldsymbol{\eta}_P) \end{aligned}$$

Therefore:

$$\begin{aligned} & \nabla_\eta^2 \psi(\boldsymbol{\eta}_P) \\ & \stackrel{1.9}{=} \int_X (\mathbf{x} - \nabla_\eta \psi(\boldsymbol{\eta}_P)) (\mathbf{x} - \nabla_\eta \psi(\boldsymbol{\eta}_P)) p_\eta(\mathbf{x}) d\mathbf{x} \\ & \stackrel{1.5}{=} \int_X (\mathbf{x} - \mathbb{E}[\mathbf{x}])^2 p_\eta(\mathbf{x}) d\mathbf{x} \\ &= \text{Var}_\eta[\mathbf{x}] \end{aligned}$$

This proves equation 1.6. Furthermore since:

$$\nabla_\eta^2 \psi(\boldsymbol{\eta}_P) = \text{Var}_\eta[\mathbf{x}] \geq 0, \forall \boldsymbol{\eta}_P \in \text{img} \eta$$

□

The Hessian matrix of ψ is positive definite and therefore ψ is convex. The convexity of ψ may therefore be used to induce a Riemannian metric by the Bregman divergence.

Lemma 2. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) . Then the Bregman divergence given by D_ψ , is the dual Kullback-Leibler divergence, such that:*

$$(1.10) \quad D_\psi[P \parallel Q] = D_{\text{KL}}^*[P \parallel Q], \forall P, Q \in \mathcal{P}$$

Proof. Let $P, Q \in \mathcal{P}$ and p, q their respectively density functions over (X, Σ_X) . By calculating:

$$(1.11) \quad \log p_\eta(\mathbf{x}) = \boldsymbol{\eta}_P \cdot \mathbf{x} - \psi(\boldsymbol{\eta}_P)$$

the Bregman divergence is derived by:

$$\begin{aligned}
& D_\psi[P \parallel Q] \\
&= \psi(\boldsymbol{\eta}_P) - \psi(\boldsymbol{\eta}_Q) \\
&\quad - \nabla_\eta \psi(\boldsymbol{\eta}_Q) \cdot (\boldsymbol{\eta}_Q - \boldsymbol{\eta}_P) \\
&= \left(\int_X (\boldsymbol{\eta}_Q \cdot \mathbf{x}) q(\mathbf{x}) d\mathbf{x} - \psi(\boldsymbol{\eta}_Q) \right) \\
&\quad - \left(\int_X (\boldsymbol{\eta}_P \cdot \mathbf{x}) q(\mathbf{x}) d\mathbf{x} - \psi(\boldsymbol{\eta}_P) \right) \\
&\stackrel{1.11}{=} \int_X q_\eta(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x} \\
&\quad - \int_X q(\mathbf{x}) \log p(\mathbf{x}) d\mathbf{x} \\
&= \int_X q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x} \\
&= D_{\text{KL}}^*[P \parallel Q]
\end{aligned}$$

Lemma 3. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) . Then the Bregman divergence given by D_ψ , induces a Riemannian metric, which is given by the Fisher information:*

$$(1.12) \quad g_{P,\psi} = \mathbb{I}[P \mid X]$$

Proof. Let $P \in \mathcal{P}$ and p the probability density function of P over (X, Σ_X) , then:

$$(1.13) \quad \nabla_\eta \log p_\eta(\mathbf{x}) = \nabla_\eta (\boldsymbol{\eta}_P \cdot \mathbf{x} - \psi(\boldsymbol{\eta}_P)) = \mathbf{x} - \nabla_\eta \psi(\boldsymbol{\eta}_P)$$

The Riemannian metric, which is induced by the Bregman divergence D_ψ is therefore given by:

$$\begin{aligned}
g_{P,\psi} &= \nabla_\eta^2 \psi(\boldsymbol{\eta}_P) \\
&\stackrel{1.9}{=} \int_X (\mathbf{x} - \nabla_\eta \psi(\boldsymbol{\eta}_P))^2 p_\eta(\mathbf{x}) d\mathbf{x} \\
&\stackrel{1.13}{=} \int_X (\nabla_\eta \log p_\eta(\mathbf{x}))^2 p_\eta(\mathbf{x}) d\mathbf{x} \\
&\stackrel{\text{def}}{=} \mathbb{I}[P_\eta \mid X]
\end{aligned}$$

Lemma 4. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) and $(X, \mathcal{P}_\eta, D_\psi)$ the Riemannian statistical manifold, given by the Bregman divergence D_ψ . Then the η -affine geodesics in $(X, \mathcal{P}_\eta, D_\psi)$ are given by exponential families.*

Proof. The η -affine geodesics in $(X, \mathcal{P}_\eta, D_\psi)$ are given by affine linear curves in the η -parametrisation. For $P, Q \in \mathcal{P}$ and $\boldsymbol{\eta}_{P,Q}(t) = (1-t)\boldsymbol{\eta}_P + t\boldsymbol{\eta}_Q$, with $t \in [0, 1]$ let $\gamma_{P,Q}(t)$ be the η -affine geodesic connecting P with Q and $d_X \gamma_{P,Q}(t)$ the probability density function of $\gamma_{P,Q}(t)$ over (X, Σ_X) . Then then representation of $d_X \gamma_{P,Q}(t)$ in the η -parametrisation is given by:

$$d_X \gamma_{P,Q}(t)(\mathbf{x}) = \exp(t(\boldsymbol{\eta}_Q - \boldsymbol{\eta}_P) \cdot \mathbf{x} + \boldsymbol{\eta}_P \cdot \mathbf{x} - \psi_\eta(t))$$

□

Let p, q be the respective probability densities of P and Q over (X, Σ_X) . A log-transformation and a subsequent substitution of $\boldsymbol{\eta}_P$ and $\boldsymbol{\eta}_Q$ by equation 1.11 yields:

$$\log d_X \gamma_{P,Q}(t)(\mathbf{x}) = (1-t) \log p(\mathbf{x}) + t \log q(\mathbf{x}) - \psi(t)$$

A further exp-transformation and subsequent integration over a measurable set $\sigma \in \Sigma$ gives:

$$\begin{aligned}
\gamma_{P,Q}(t)[\sigma] &= \int_\sigma \exp((1-t) \log p(\mathbf{x})) d\mathbf{x} \\
&\quad \cdot \int_\sigma \exp(t \log q(\mathbf{x}) - \psi(t)) d\mathbf{x}
\end{aligned}$$

For varying $P, Q \in \mathcal{P}$ this yields a generic representation of η -affine geodesics in $(X, \mathcal{P}_\eta, D_\psi)$, by are exponential families with respect to the curve parameter t . □

Lemma 5. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) and $(X, \mathcal{P}_\eta, D_\psi)$ the Riemannian statistical manifold, given by the Bregman divergence D_ψ . Then the η -affine geodesics in $(X, \mathcal{P}_\eta, D_\psi)$ are flat with respect to the Fisher information.*

□

2. DUAL AFFINE STRUCTURE OF EXPONENTIAL FAMILIES

In the purpose, to study the structure, obtained by a Legendre transformation a further parametric family is introduced, that is shown to cover this dual structure. This parametric family is the mixture family.

Definition (Mixture family). *Let*

$$(\Omega, \mathcal{F}_\theta) \in \text{ob}(\mathbf{Stat})$$

be a statistical model over a measurable space (Ω, Σ_Ω) . Then (Ω, \mathcal{F}) is a mixture family if and only if there is an invertible function $w : \text{dom}\theta \rightarrow \mathbb{R}^{n+1}$ with $w_i(\theta_p) > 0, \forall i$ and $\sum_{i=0}^n w_i(\theta_p) = 1, \forall \theta_p$ and $n+1$ pairwise independent probability distributions Q_i over (Ω, Σ_Ω) , such that for all $P_\theta \in \mathcal{F}_\theta$:

$$(2.1) \quad P_\theta[\sigma] = \sum_{i=0}^n w_i(\theta_p) Q_i[\sigma], \forall \sigma \in \Sigma_\Omega$$

The normalization condition can be used to restrict the number of parameters, by the definition:

$$(2.2) \quad R(\theta_p)[\sigma] = \left(1 - \sum_{i=1}^n w_i(\theta_p)\right) Q_0[\sigma]$$

Therefore:

$$P_\theta[\sigma] = \sum_{i=1}^n w_i(\theta_p) Q_i[\sigma] + R(\theta_p)[\sigma]$$

This transformation is a globally invertible Markov morphism, and its restriction to (Ω, \mathcal{F}) yields a statistical isomorphism $\mathfrak{T} \in \text{iso}(\mathbf{Stat})$ to a statistical model $(X, \mathcal{P}) := \text{img}\mathfrak{T}$. Then $\mu := w \circ \theta^{-1}$ is an identifiable parametrisation of (X, \mathcal{P}) and since w defines a probability distribution over θ it may be regarded as the expected value $E_\theta[\mathbf{x}]$ with respect to P_θ . By the definition of $\varphi := -w^{-1} \circ R \circ w$ it follows that:

$$(2.3) \quad P_\mu[\sigma] = \boldsymbol{\mu}_P \cdot \mathbf{Q}[\sigma] - \varphi(\boldsymbol{\mu}_P)[\sigma]$$

Without loss of generality any mixture family may therefore be assumed to be given by equations 2.3.

This representation is termed the canonical form of a mixture family and the parametrisation μ the expectation parametrisation.

Definition (Expectation parametrisation). *Let*

$$(X, \mathcal{P}_\theta) \in \text{ob}(\mathbf{Stat})$$

Then a parametrisation μ with $\text{dom}\mu \subseteq \mathbb{R}^n$, which is given by $\boldsymbol{\mu}_P = E_\theta[\mathbf{x}]$, where $E_\theta[\mathbf{x}]$ denotes the vectorial expectation of \mathbf{x} with respect to P_θ , is termed an expectation parametrisation with respect to θ and parameter vectors $\boldsymbol{\mu}_P \in \text{dom}\mu$ are termed expectation parameters.

Lemma 6. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) and φ the negative entropy $-\text{H}[P_\eta | X]$. Then the dual parametrisation η^* is given by the expectation parametrisation μ and the Legendre dual function ψ^* by φ , such that:*

$$(2.4) \quad \boldsymbol{\eta}_P^* = \boldsymbol{\mu}_P$$

$$(2.5) \quad \psi^*(\boldsymbol{\eta}_P^*) = \varphi(\boldsymbol{\mu}_P)$$

Proof. Let $P_\eta \in \mathcal{P}$ and p_η the density function of P_η over (X, Σ_X) . Then from equation 1.5 it follows, that:

$$\boldsymbol{\eta}_P^* = \nabla_\eta \psi(\boldsymbol{\eta}_P) \stackrel{1.5}{=} E_\eta[\mathbf{x}] \stackrel{\text{def}}{=} \boldsymbol{\mu}_P$$

the dual parametrisation $\boldsymbol{\eta}_P^*$ directly follows from .

The Legendre dual function ψ^* is derived by:

$$\begin{aligned} \psi^*(\boldsymbol{\eta}_P^*) &\stackrel{??}{=} \boldsymbol{\eta}_P \cdot \nabla_\eta \psi(\boldsymbol{\eta}_P) - \psi(\boldsymbol{\eta}_P) \\ &\stackrel{1.7}{=} \int_X (\boldsymbol{\eta}_P \cdot \mathbf{x}) p_\eta(\mathbf{x}) d\mathbf{x} - \psi(\boldsymbol{\eta}_P) \int_X p_\eta(\mathbf{x}) d\mathbf{x} \\ &= \int_X p_\eta(\mathbf{x}) (\boldsymbol{\eta}_P \cdot \mathbf{x} - \psi(\boldsymbol{\eta}_P)) d\mathbf{x} \\ &\stackrel{1.4}{=} \int_X p_\eta(\mathbf{x}) \log p_\eta(\mathbf{x}) d\mathbf{x} \\ &= -\text{H}[P_\eta | X] \end{aligned}$$

□

Lemma 7. *Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) . Then the*

The Bregman divergence, given by the Legendre dual function φ is the Kullback-Leibler divergence:

$$D_\varphi[P \parallel Q] = D_{\text{KL}}[P \parallel Q]$$

Proof. From lemma ??, equation ?? it follows, that:

$$\begin{aligned} D_\varphi[P \parallel Q] &\stackrel{??}{=} D_{\varphi^*}[Q_\mu^* \parallel P_\mu^*] \\ &\stackrel{\text{def}}{=} D_\psi[Q_\eta \parallel P_\eta] \\ &\stackrel{1,10}{=} D_{\text{KL}}[P \parallel Q] \end{aligned}$$

□

Lemma 8. Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) . Then the Bregman divergence D_φ of the Legendre dual function $\varphi = \psi^*$, induces a Riemannian metric, which is given by the inverse Fisher information:

$$(2.6) \quad g_{P,\varphi} = \mathbb{I}[P \mid X]^{-1}$$

Proof. By applying theorem ?? the Bregman divergence $D_\varphi = D_{\psi^*}$ induces the dual Riemannian metric $g_{P,\psi}^*$, which by definition is inverse to the Riemannian metric, induced by D_ψ , such that $g_{P,\varphi} = g_{P,\psi}^{-1}$, $\forall P \in \mathcal{P}$. From lemma 3 it follows, that $g_{P,\varphi} = \mathbb{I}[P \mid X]^{-1}$. □

Lemma 9. Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) and $(X, \mathcal{P}, D_\varphi)$ the Riemannian statistical manifold, given by the Bregman divergence D_φ of the Legendre dual function $\varphi = \psi^*$. Then the μ -affine geodesics in $(X, \mathcal{P}_\mu, D_\psi)$ are given by mixture families.

Proof. μ -affine geodesics in $(X, \mathcal{P}_\mu, D_\psi)$ are given by affine linear curves in the μ -parametrisation. For $P, Q \in \mathcal{P}$ and $\mu_{P,Q}(t) = (1-t)\mu_P + t\mu_Q$, with $t \in [0, 1]$ let $\gamma_{P,Q}(t)$ be the μ -affine geodesic connecting P with Q and $d_x \gamma_{P,Q}(t)$ the probability density of $\gamma_{P,Q}(t)$ over (X, Σ_X) , then:

$$d_x \gamma_{P,Q}(t)(\mathbf{x}) = (1-t)\mu(\mathbf{x}) + t\mu_Q(\mathbf{x})$$

An integration over σ yields:

$$\gamma_{P,Q}(t) = \int_\sigma ((1-t)p(\mathbf{x}) + tq(\mathbf{x})) d\mathbf{x}$$

This is a mixture of probability distributions with respect to a mixing parameter t . □

Lemma 10. Let ψ be the cumulant generating function of an exponential family (X, \mathcal{P}_η) . Then the μ -affine geodesics are flat with regard to the Riemannian metric, induced by the Bregman divergence D_φ of the Legendre dual function $\varphi = \psi^*$.

3. Dually Flat Structure

Theorem 11 (Structure of Exponential Families). Let (X, \mathcal{P}) be an exponential family. Then there exists a Bregman divergence D_ψ such that $(X, \mathcal{P}_\eta, D_\psi)$ is a dually flat statistical manifold with respect to the Riemannian metric, induced by D_ψ .

Proof. Let η be the natural parametrisation and ψ the cumulant generating function of (X, \mathcal{P}) . Let further be D_ψ the Bregman divergence over (X, \mathcal{P}) with respect to ψ , then $(X, \mathcal{P}_\eta, D_\psi)$ is a Riemannian statistical manifold with a Bregman divergence D_ψ . By lemma 3 it follows that η is an affine parametrisation and by lemma 5 that the η -affine geodesics are flat with respect to the Riemannian metric, induced by D_ψ . Let μ be the expectation parametrisation of (X, \mathcal{P}) with respect to η , then by lemma 1 it follows, that $\mu = \eta^*$, by lemma 8, that μ is an affine parametrisation of $(X, \mathcal{P}, D_{\psi^*})$ and by lemma 10 that the μ -affine geodesics are flat with respect to the Riemannian metric, induced by D_φ , where $\varphi = \psi^*$. Therefore the conditions of lemma ?? are satisfied and $(X, \mathcal{P}_\xi, D_\psi)$ is a dually flat statistical manifold. □

Together the primary and dual affine structure of an exponential family induce a dually flat structure, which is characterized by the η -affine and μ -affine geodesics, with respect to the Fisher information metric and its dual metric. Thereby the η -affine geodesics are represented by exponential families over the curve parameter t and the μ -affine

geodesics by mixture families. This relationship allows a characterisation of the intrinsic dually flat structure, which is independent of its parametrisation. This structure is given by an *e-affine structure*, that preserves the exponential family representation within its primary affine structure and an *m-affine structure* that preserves the dual representation within the dual affine structure. Therefore geodesics and geodesic projections in the *e-affine structure* are respectively termed *e-geodesics*, denoted by γ_e and *e-affine projections*, denoted by π_e . Furthermore the geodesics and geodesic projections in the *m-affine structure* are respectively termed *m-geodesics*, denoted by γ_m and *m-affine projections*, denoted by π_m . With respect to submanifolds, a smooth submanifold is termed *e-flat* if it has a linear embedding within the *e-affine structure* and *m-flat* if it has a linear embedding within the *m-affine structure*.

Corollary 12. *Let (X, \mathcal{P}) be an exponential family and $P \in \mathcal{P}$. Then the geodesic projection of P to an *m-flat* submanifold is uniquely given by an *e-affine projection* π_e and the geodesic projection of P to an *e-flat* submanifold is uniquely given by an *m-affine projection* π_m .*

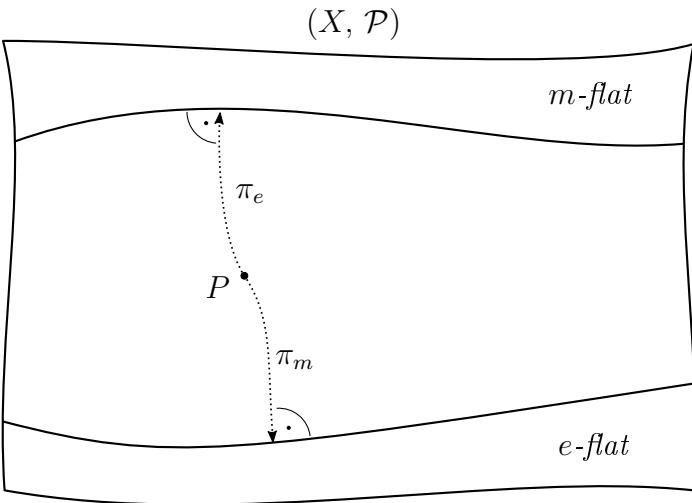


FIGURE 3.1. Unique projection in Exponential Families

Proof. Let (X, \mathcal{P}) be an exponential family. Then theorem 11 states, that the structure of (X, \mathcal{P}) is given by a dually flat statistical manifold $(X, \mathcal{P}_\eta, D_\psi)$, where the Riemannian metric is induced by a Bregman divergence D_ψ with respect to the natural parametrisation η . Let (X, \mathcal{Q}) be an *m-flat* submanifold, then (X, \mathcal{Q}) is flat with regard to the Riemannian metric, induced by the expectation parametrisation and therefore flat with respect to D_{ψ^*} . Conversely let (X, \mathcal{S}) be an *e-flat* submanifold, then (X, \mathcal{Q}) is flat with regard to the Riemannian metric, induced by the natural parametrisation and therefore flat with respect to D_ψ . Therefore the conditions of corollary ?? are satisfied, which proves the corollary. \square

4. MAXIMUM ENTROPY ESTIMATION IN EXPONENTIAL FAMILIES

The sample space (X, Σ) of a statistical model (X, \mathcal{P}) is generated by a statistic T , that induces a probability distribution P_X from the probability space of an underlying statistical population (Ω, \mathcal{F}, P) . To this end also the sample space may be regarded as a probability space, whereat the occurrence of the probability distribution P_X is hypothetical.

Lemma 13. *Let (X, \mathcal{P}_η) be an exponential family over a sample space (X, Σ) , and P_U the uniform distribution over (X, Σ) . Then $P_U \in \mathcal{P}$.*

Proof. Let μ be a σ -finite reference measure over (X, Σ) , then the probability density u of the uniform distribution is given by:

$$u_X(x) := \begin{cases} \frac{1}{\mu(X)} & x \in X \\ 0 & x \notin X \end{cases}$$

Let η be the canonical parametrisation of (X, \mathcal{P}) , then the densities of any $P \in \mathcal{P}$ may be written as:

$$p_\eta(\mathbf{x}) = \exp(\boldsymbol{\eta}_P \cdot \mathbf{x} - \psi(\boldsymbol{\eta}_P))$$

Where the cumulative generating function $\psi(\boldsymbol{\eta}_P)$ is given by:

$$\psi(\boldsymbol{\eta}_P) = \log \int_X \exp(\boldsymbol{\eta}_P \cdot \mathbf{x}) d\mu(\mathbf{x})$$

Let $\boldsymbol{\eta}_P = 0$, then:

$$\begin{aligned} p_\eta(\mathbf{x}) &= \exp(0 \cdot \mathbf{x} - \psi(0)) \\ &= \exp\left(\log \int_X d\mu(\mathbf{x})\right)^{-1} \\ &= \mu(X)^{-1} \end{aligned}$$

This is the density of the uniform distribution over (X, Σ) . \square

Lemma 14. *Let (X, Σ) be a measurable space and P_U the uniform distribution over (X, Σ) . Then let P be an arbitrary probability distribution over (X, Σ) , then:*

$$H[P_U | X] \geq H[P | X]$$

Proof. Let u_X be the probability density of P_U , then the entropy of P_U over (X, Σ) is:

$$\begin{aligned} H[P_U | X] &= - \int_X u_X(x) \log u_X(x) d\mu(x) \\ &= - \int_X \mu(X)^{-1} \log \mu(X)^{-1} d\mu(x) \\ &= \log \mu(X)^{-1} \end{aligned}$$

Let P be an arbitrary probability distribution over (X, Σ) with density p , then:

$$\begin{aligned} D_{\text{KL}}[P \parallel P_U] &= \int_X p(x) \log \frac{p(x)}{u_X(x)} d\mu(x) \\ &= \int_X p(x) \log p(x) d\mu(x) \\ &\quad - \int_X p(x) \log u_X(x) d\mu(x) \\ &= -H[P | X] - \log \mu(X)^{-1} \\ &= -H[P | X] + \mathcal{H}[P_U | X] \geq 0 \end{aligned}$$

Therefore:

$$\mathcal{H}[P_U | X] \geq \mathcal{H}[P | X], \forall P$$

\square

Lemma 15. *Let (X, \mathcal{P}) be an exponential family over a sample space (X, Σ) . Then a maximum entropy estimation of (X, \mathcal{P}) is given by the uniform probability distribution over (X, \mathcal{P}) .*

Proof. From lemma 13 it follows, that $P_U \in \mathcal{P}$. Furthermore lemma 14 proves that P_U maximizes the entropy among all $P \in \mathcal{P}$. \square

Theorem 16. *Let (X, \mathcal{P}) be an exponential family over a sample space (X, Σ) and (X, \mathcal{Q}) a smooth submanifold, then a maximum entropy estimation of (X, \mathcal{Q}) is given by a geodesic projection of the uniform probability distribution over (X, \mathcal{P}) to (X, \mathcal{Q}) .*

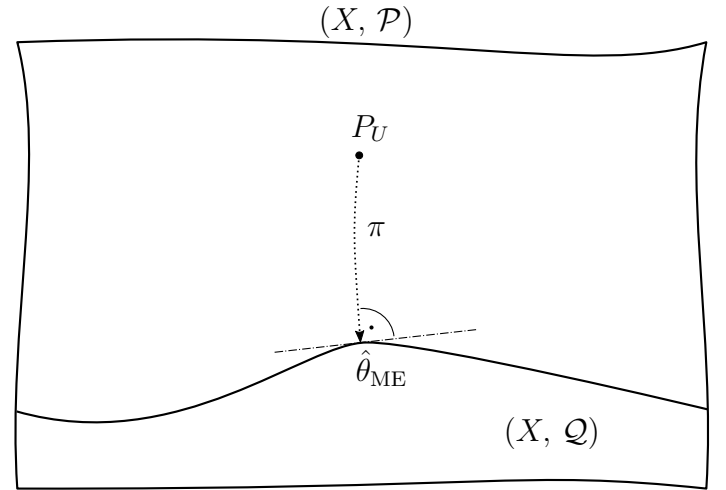


FIGURE 4.1. ME estimation in Exponential Families

Proof. [todo] \square

By assuming a given event $\sigma \in \Sigma$ within a sample space (X, Σ) , the principle of maximum entropy emphasizes a probability distribution, that minimizes additional assumptions. Then lemma 15 states, that the maximum entropy estimation of a single observation within the set of all probability distributions is given by the uniform probability distribution over this observation, such that:

$$u_\sigma(x) := \begin{cases} \frac{1}{\mu(\sigma)} & , x \in \sigma \\ 0 & , x \notin \sigma \end{cases}$$

The dispensation of any additional knowledge except the observation itself determines the uniform probability distribution as the empirical probability of a single observation. This shall be extended to repeated observations. Let $\sigma = (\sigma_i)_{i \in I}$ be a repeated observation in (X, Σ) , then the density function of a finite measure over (X, Σ) is given by the arithmetic mean of the uniform distributions of the individual single observations:

$$f_\sigma(x) = \frac{1}{|I|} \sum_{i \in I} u_{\sigma_i}(x) = \frac{1}{|I|} \sum_{i \in I} \frac{\delta_x(\sigma_i)}{\mu(\sigma_i)}$$

Where μ is a σ -finite reference measure and δ the Dirac measure and defined by:

$$\delta_x(\sigma) = \begin{cases} 1 & , x \in \sigma \\ 0 & , x \notin \sigma \end{cases}$$

Then f_σ is a probability density function over (X, Σ) , since $f_\sigma(x) > 0, \forall x \in X$ and:

$$\begin{aligned} \int_X f_\sigma(x) d\mu(x) &= \int_X \frac{1}{|I|} \sum_{i \in I} \frac{\delta_x(\sigma_i)}{\mu(\sigma_i)} d\mu(x) \\ &= \frac{1}{|I|} \sum_{i \in I} \frac{1}{\mu(\sigma_i)} \left(\int_X \delta_x(\sigma_i) d\mu(x) \right) \\ &= \frac{1}{|I|} \sum_{i \in I} \frac{\mu(X \cap \sigma_i)}{\mu(\sigma_i)} = 1 \end{aligned}$$

Furthermore the assumptions given by f_σ are equal the knowledge which is given by the repeated observation σ . This determines f_σ as the density of an empirical probability distribution.

Definition (Empirical probability distribution). *Let (X, Σ) be a measurable space, $\sigma = (\sigma_i)_{i \in I}$ a repeated observation in (X, Σ) and μ a σ -finite reference measure over (X, Σ) . Then the empirical probability distribution of σ over (X, Σ) is given by:*

$$P_\sigma[A] := \int_A \frac{1}{|I|} \sum_{i \in I} \frac{\delta_x(\sigma_i)}{\mu(\sigma_i)} d\mu(x), \forall A \in \Sigma$$

Proposition 17. *Let (X, Σ) be a sample space, P_X be observable distribution of (X, Σ) and $\sigma(n)$ =*

$(\sigma_i)_{i \leq n}$ the partial sequences of a repeated observation $\sigma = (\sigma_i)_{i \in \mathbb{N}}$ in (X, Σ) . Then the sequence of the empirical probability distributions $P_{\sigma(n)}$ converges to P_X as $n \rightarrow \infty$.

Proof. Let p_X be the probability density function of P_X . Then due to the strong law of large numbers it follows, that:

$$(4.1) \quad \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i \in 1}^n \frac{\delta_x(\sigma_i)}{\mu(\sigma_i)} \stackrel{a.s.}{=} E[\delta_x(y)] = \int_X \delta_x(y) dp_X(y)$$

Let $A \in \Sigma$, then the limit of the empirical probability distributions $P_n[A]$ is given by:

$$\begin{aligned} &\lim_{n \rightarrow \infty} P_n[A] \\ &= \lim_{n \rightarrow \infty} \int_A \frac{1}{n} \sum_{i \in 1}^n \frac{\delta_{\{x\}}(\sigma_i)}{\mu(\sigma_i)} d\mu(x) \\ &= \int_A \left(\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i \in 1}^n \frac{\delta_{\{x\}}(\sigma_i)}{\mu(\sigma_i)} \right) d\mu(x) \\ &\stackrel{a.s.}{=} \int_A \int_X \delta_{\{x\}}(y) dp_X(y) d\mu(x) \\ &= \int_A p_X(x) d\mu(x) \\ &= P_X[A] \end{aligned}$$

□

5. MAXIMUM LIKELIHOOD ESTIMATION IN EXPONENTIAL FAMILIES

Lemma 18. *Let (X, \mathcal{Q}) be a statistical model over a sample space (X, Σ) and σ a finite repeated observation in (X, Σ) . Then the MLE has the following representation:*

$$(5.1) \quad \hat{\theta}_{ML} \in \arg \max_{\theta} \sum_{i=1}^n \log L[Q_\theta | \sigma_i]$$

Proof. Since the log transformation is strictly monotonous over $\text{img} L \subseteq [0, 1]$ it directly follows, that:

$$\arg \max_{\theta} L[Q_\theta | \sigma] = \arg \max_{\theta} \log L[Q_\theta | \sigma]$$

Furthermore due to pairwise independence of the individual observations are it follows, that:

$$\log L[Q_\theta \mid \sigma] = \log \prod_{i=1}^n L[Q_\theta \mid \sigma_i] = \sum_{i=1}^n \log L[Q_\theta \mid \sigma_i]$$

And therefore:

$$\begin{aligned} \hat{\theta}_{\text{ML}} &\in \arg \max_{\theta} L[Q_\theta \mid \sigma] \\ &= \arg \max_{\theta} \sum_{i=1}^n \log L[Q_\theta \mid \sigma_i] \end{aligned}$$

Lemma 19. *Let (X, \mathcal{Q}) be a statistical model over a sample space (X, Σ) and σ a finite repeated observation in (X, Σ) . Let further be p_σ the empirical probability density with respect to σ . Then the MLE has the following representation:*

$$(5.2) \quad \hat{\theta}_{\text{ML}} \in \arg \max_{\theta} \int_X p_\sigma(x) \log q_\theta(x) d\mu(x)$$

Proof. By substitution of the empirical probability density $p_\sigma(x)$ it follows that:

$$\begin{aligned} (5.3) \quad &\int_X p_\sigma(x) \log q_\theta(x) d\mu(x) \\ &= \int_X \left(\frac{1}{n} \sum_{i \in I} \frac{1}{\mu(\sigma_i)} \delta_{\{x\}}(\sigma_i) \right) \log q_\theta(x) d\mu(x) \\ &= \frac{1}{n} \sum_{i \in I} \frac{1}{\mu(\sigma_i)} \int_{\sigma_i} \log q_\theta(x) d\mu(x) \\ &= \frac{1}{n} \sum_{i \in I} \frac{1}{\mu(\sigma_i)} (\mu(\sigma_i) \log L[Q_\theta \mid \sigma_i] - \mu(\sigma_i)) \\ &= \frac{1}{n} \sum_{i \in I} \log L[Q_\theta \mid \sigma_i] - 1 \end{aligned}$$

The maximization of equation 5.3 with respect to θ therefore yields the following identity:

$$\begin{aligned} &\arg \max_{\theta} \int_X p_\sigma(x) \log q_\theta(x) d\mu(x) \\ &= \arg \max_{\theta} \left(\frac{1}{n} \sum_{i \in I} \log L[Q_\theta \mid \sigma_i] - 1 \right) \\ &= \arg \max_{\theta} \sum_{i \in I} \log L[Q_\theta \mid \sigma_i] \end{aligned}$$

By lemma 18, equation 5.1 it follows, that:

$$\hat{\theta}_{\text{ML}} \in \arg \max_{\theta} \int_X p_\sigma(x) \log q_\theta(x) d\mu(x)$$

□

Theorem 20. *Let (X, \mathcal{P}) be an exponential family over a sample space (X, Σ) . Let further be (X, \mathcal{Q}) a smooth submanifold of (X, \mathcal{P}) and σ a repeated observation in (X, Σ) . Then a maximum likelihood estimation of (X, \mathcal{Q}) respective to σ is given by the geodesic projection of the empirical probability P_σ to (X, \mathcal{Q}) in (X, \mathcal{P}) .*

□

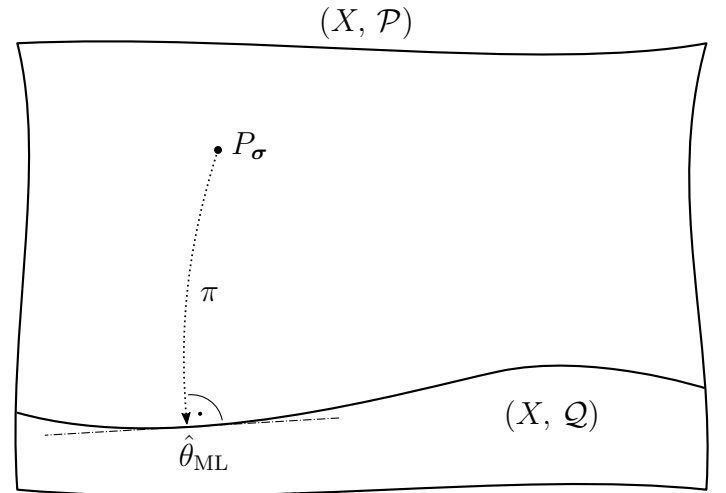


FIGURE 5.1. ML estimation in Exponential Families

Proof. Let (X, \mathcal{P}_η) be an exponential family over a sample space (X, Σ) and (X, \mathcal{Q}) a smooth submanifold of (X, \mathcal{P}) . Then there exists a Bregman divergence D_ψ , such that $(X, \mathcal{P}_\eta, D_\psi)$ is a dually flat statistical manifold and η is the e -affine parametrisation of $(X, \mathcal{P}_\eta, D_\psi)$. Then $(X, \mathcal{Q}_\eta, D_\psi)$ is a smooth Riemannian submanifold of $(X, \mathcal{P}_\eta, D_\psi)$ with respect to the induced Riemannian metric D_ψ . Let σ be a repeated observation over (X, Σ) and P_σ its empirical probability distribution.

Then P_σ is given in expectation parameters in (X, Σ) and therefore in an m -affine parametrisation within Riemannian Manifold $(X, \mathcal{P}_\eta, D_\psi)$. By

applying the projection theorem the geodesic projection of P_σ to $(X, \mathcal{Q}_\eta, D_\psi)$, equals the dual affine projection, and therefore by a point $Q \in \mathcal{Q}$, that minimizes the Bregman divergence $D_\psi[Q \parallel P_\sigma]$. The geodesic distance is therefore given by:

$$\begin{aligned}
& d(P_\sigma, Q) \\
&= D_\psi[Q \parallel P_\sigma] \\
&= D_{\text{KL}}[P_\sigma \parallel Q] \\
&= \int_X p_\sigma(x) \log \frac{p_\sigma(x)}{q(x)} d\mu(x) \\
&= \int_X p_\sigma(x) \log p_\sigma(x) d\mu(x) \\
&\quad - \int_X p_\sigma(x) \log q(x) d\mu(x) \\
&= -H[P_\sigma \mid X] - \int_X p_\sigma(x) \log q(x) d\mu(x)
\end{aligned}$$

The minimization of $d(P_\sigma, Q)$ with respect to the natural parametrisation η therefore yields the following identity:

$$(5.4) \quad \arg \min_{\eta} d(P_\sigma, Q_\eta) = \arg \max_{\eta} \int_X p_\sigma(x) \log q_\eta(x) d\mu(x)$$

By equation 5.2 and lemma, equation 5.4 it follows, that:

$$\begin{aligned}
\hat{\theta}_{\text{ML}} &\stackrel{5.2}{\in} \arg \max_{\eta} \int_X p_\sigma(x) \log q_\eta(x) d\mu(x) \\
&\stackrel{5.4}{=} \arg \min_{\eta} d(P_\sigma, Q_\eta)
\end{aligned}$$

6. LATENT VARIABLE MODELS

Exponential families, as introduced in the previous sections, statistically relate random variables over a common statistical population by their common probability distribution in the sample space. In many cases however the intrinsic structure of this relationship has a natural decomposition by the introduction of latent random variables, that are not directly observable from the statistical population but assumed to affect the observations. This is of

particular importance for the modelling of statistical populations with complex network structures. In this case the properties of the network may be incorporated by the conditional transition probabilities between observable and latent random variables.

In completely observable statistical models, the probability distributions may be estimated by the empirical probability distributions of repeated observations. In latent variable models however the conditional transition probabilities $p(v \mid h)$ and $p(h \mid v)$ between the observables $v \in V$ and the latent variables $h \in H$ in general prevent this inference. The only exception is given if $p(v \mid h)$ and $p(h \mid v)$ are uniform distributed, such that for any given v any h has the same probability with respect to v and vice versa. In this case estimations decompose into independent estimations of the observable variables and the latent variables. If the conditional transition probabilities, however are not uniform distributed, they have to be taken into account for estimations. This also applies to empirical distributions. Let $\sigma(n) = (\sigma_i)_{i \leq n}$ be the partial sequences of a repeated observation $\sigma = (\sigma_i)_{i \in \mathbb{N}}$ in (V, Σ_v) , then by proposition 17 it follows, that the empirical probabilities $P_{\sigma(n)}$ converge in distribution to the true probability distribution P_V of (V, Σ_v) . Since P_V however is the marginal distribution of the observables in (X, Σ) the common empirical probabilities over (X, Σ) are constituted by an empirical probability of a repeated observation and a conditional transition probability. The probability density p_σ of an empirical probability over (X, Σ) is therefore given by:

$$p_\sigma(x) = p_\sigma(v, h) = p_\sigma(v)p(h \mid v), \forall x \in X$$

In the presence of continuous variables it is useful to restrict the empirical probability distributions to “non pathological” cases. This restriction defines statistical model with respect to empirical observations.

Definition (Empirical model). *Let (X, Σ) be a partially observable measurable space with $X = V \times H$. Then a statistical model (X, \mathcal{E}) is termed an empirical model over (X, Σ) if \mathcal{E} comprises all empirical probability distributions over (X, Σ) , which are constituted by a finite repeated observation and a conditional transition probability of a given set \mathcal{T} . If \mathcal{T} is the set of all absolutely continuous conditional transition probabilities, then (X, \mathcal{E}) is termed an absolutely continuous empirical model.*

7. EXPONENTIAL FAMILIES WITH LATENT VARIABLES

Let (X, \mathcal{P}) be an exponential family over a partially observable measurable space (X, \mathcal{P}) . Then due to theorem 11 the structure of (X, \mathcal{P}) is that of a dually flat manifold such that there exists a parametrisation η and a convex function ψ , that allow to regard (X, \mathcal{P}) as a dually flat statistical manifold, given by $(X, \mathcal{P}_\eta, D_\psi)$. In the purpose of observation based estimations in the presence of latent variables, the obstacle that has to be taken is the extension of $(X, \mathcal{P}_\eta, D_\psi)$ to a dually flat embedding space (X, \mathcal{U}, D) , that covers $(X, \mathcal{P}_\eta, D_\psi)$ as well as the empirical model (X, \mathcal{E}) . For arbitrary empirical models however this embedding does generally not exist, for which (X, \mathcal{E}) is assumed to be absolutely continuous. Then (X, \mathcal{E}) is generally an infinite dimensional exponential family.

Lemma 21. *Let (X, \mathcal{E}) be an absolutely continuous empirical model over a partially observable measurable space (X, Σ) . Then (X, \mathcal{E}) is an infinite dimensional exponential family and its probability densities are given by:*

$$p_\sigma(\mathbf{v}, \mathbf{h}) = \frac{\exp \int_H \eta_s(\mathbf{v}, \mathbf{r}) \delta(\mathbf{h} - \mathbf{r}) d\mathbf{r}}{\exp \psi_s(\eta_s(\mathbf{v}, \mathbf{h}))}$$

where $\mathbf{v} \in \mathbb{R}^k$ and $\mathbf{h} \in \mathbb{R}^l$ respectively denote the observable and latent variables, $\eta_s(\mathbf{v}, \mathbf{h})$ scalar coefficients and ψ_s the cumulant generating function,

given by:

$$(7.1) \quad \psi_s(\eta_s(\mathbf{v}, \mathbf{h})) = \log \int_{\mathbb{R}^l} \exp(\eta_s(\mathbf{v}, \mathbf{r})) d\mathbf{r}$$

Proof. Due to the definition of an empirical model the probability density p_σ of any $P \in \mathcal{E}$ may be written as:

$$(7.2) \quad p_\sigma(\mathbf{v}, \mathbf{h}) = \frac{1}{n} \sum_{i=1}^n \delta(\mathbf{v} - \mathbf{s}_i) p(\mathbf{h} | \mathbf{s}_i)$$

Furthermore any conditional transition probability $p(\mathbf{h} | \mathbf{v})$ is given by:

$$(7.3) \quad p(\mathbf{h} | \mathbf{v}) = \int_H \delta(\mathbf{h} - \mathbf{r}) p(\mathbf{r} | \mathbf{v}) d\mathbf{r}$$

Therefore by equation 7.2 and 7.3 it follows, that:

$$(7.4) \quad p_s(\mathbf{v}, \mathbf{h}) = \frac{1}{n} \sum_{i=1}^n \delta(\mathbf{v} - \mathbf{s}_i) \int_{\mathbb{R}^l} \delta(\mathbf{h} - \mathbf{r}) p(\mathbf{r} | \mathbf{s}_i) d\mathbf{r}$$

Since $p(\mathbf{h} | \mathbf{v})$ are absolutely continues equation 7.4 may be rewritten to:

$$p_s(\mathbf{v}, \mathbf{h}) = \int_H \left(\frac{1}{n} \sum_{i=1}^n \delta(\mathbf{v} - \mathbf{s}_i) p(\mathbf{r} | \mathbf{s}_i) \right) \delta(\mathbf{h} - \mathbf{r}) d\mathbf{r}$$

By the substitution

$$(7.5) \quad \mu_s(\mathbf{v}, \mathbf{r}) = \frac{1}{n} \sum_{i=1}^n \delta(\mathbf{v} - \mathbf{s}_i) p(\mathbf{r} | \mathbf{s}_i)$$

it follows, that the the empirical probabilities in \mathcal{E} may be written as a mixture with mixing coefficients $\mu_s(\mathbf{v}, \mathbf{r})$:

$$(7.6) \quad p_s(\mathbf{v}, \mathbf{h}) = \int_H \mu_s(\mathbf{v}, \mathbf{r}) \delta(\mathbf{h} - \mathbf{r}) d\mathbf{r}$$

This shows, that \mathcal{E} is an infinite dimensional mixture family. By a further transformation:

$$\eta_s(\mathbf{v}, \mathbf{h}) = \log \mu_s(\mathbf{v}, \mathbf{h}) + \psi_s$$

a dual representation of equation 7.6 is obtained, with:

$$(7.7) \quad p_s(\mathbf{v}, \mathbf{h}) = \frac{\exp \int_{\mathbb{R}^l} \eta_s(\mathbf{v}, \mathbf{r}) \delta(\mathbf{h} - \mathbf{r}) d\mathbf{r}}{\exp \psi_s(\eta_s(\mathbf{v}, \mathbf{h}))}$$

This shows, that (X, \mathcal{E}) is also an infinite dimensional exponential family with natural variables $\eta_s(\mathbf{v}, \mathbf{r})$

and the cumulative generating function is given by

$$\psi_s(\eta_s(\mathbf{v}, \mathbf{h})) = \log \int_{\mathbb{R}^l} \exp(\eta_s(\mathbf{v}, \mathbf{r})) d\mathbf{r}$$

□

Lemma 22. *Let (X, \mathcal{P}) be an exponential family over a partially observable measurable space (X, Σ) and (X, \mathcal{E}) an absolutely continuous empirical model over (X, Σ) . Then there exists a dually flat statistical manifold (X, \mathcal{U}, D) , that covers (X, \mathcal{P}) and (X, \mathcal{E}) as dually flat submanifolds.*

Proof. With respect to the partially observable measurable space (X, Σ) any $p \in \mathcal{P}$ may be written as $p(\mathbf{x}) = p(\mathbf{v}, \mathbf{h})$ and any $p_s \in \mathcal{E}$ as $p_s(\mathbf{x}) = p_s(\mathbf{v}, \mathbf{h})$. Let \mathcal{U} be given by:

$$\mathcal{U} = \{q \mid q(\mathbf{v}, \mathbf{h}) = p(\mathbf{v}, \mathbf{h})p_s(\mathbf{v}, \mathbf{h}), p \in \mathcal{P}, p_s \in \mathcal{E}\}$$

Since (X, \mathcal{P}) is an exponential family it has a natural parametrisation $\boldsymbol{\eta}_{\mathcal{P}}$ and due to Lemma 21 the continuous empirical model (X, \mathcal{E}) is an infinite dimensional exponential family with natural coefficients $\boldsymbol{\eta}_{\mathcal{E}} = (\eta_s(\mathbf{v}, \mathbf{h})_{v,h})^T$. Then a parametrisation of (X, \mathcal{U}) is given by:

$$\boldsymbol{\eta} = (\boldsymbol{\eta}_{\mathcal{P}}, \boldsymbol{\eta}_{\mathcal{E}})^T$$

Let further be $\psi_{\mathcal{P}}$ the cumulant generating function of (X, \mathcal{P}) and $\psi_{\mathcal{E}}$ the cumulant generating function of (X, \mathcal{E}) , then $\psi_{\mathcal{P}}$ and $\psi_{\mathcal{E}}$ are convex functions and therefore a convex function over $\boldsymbol{\eta}$ is given by:

$$\psi(\boldsymbol{\eta}) = \psi_{\mathcal{P}}(\boldsymbol{\eta}_{\mathcal{P}}) + \psi_{\mathcal{E}}(\boldsymbol{\eta}_{\mathcal{E}})$$

This allows the definition of a Bregman divergence D_{ψ} , such that D_{ψ} induces Riemannian metric over (X, \mathcal{U}) . By substitution of equation 7.7 it follows that the application of $\boldsymbol{\eta}$ to (X, \mathcal{U}) yields a parametric representation, which is given by:

$$q_{\boldsymbol{\eta}}(\mathbf{v}, \mathbf{h}) = \exp \left(\int_{\mathbb{R}^l} \eta_s(\mathbf{v}, \mathbf{r}) \delta(\mathbf{h} - \mathbf{r}) d\mathbf{r} + \boldsymbol{\eta}_{\mathcal{P}} \cdot (\mathbf{v}, \mathbf{h})^T - \psi(\boldsymbol{\eta}) \right)$$

This shows that $(X, \mathcal{U}_{\boldsymbol{\eta}})$ is an exponential family and furthermore, that $(X, \mathcal{U}_{\boldsymbol{\eta}}, D_{\psi})$ is a dually flat statistical manifold, that covers (X, \mathcal{P}) and (X, \mathcal{E}) as smooth submanifolds. Since the projections $\boldsymbol{\eta} \rightarrow \boldsymbol{\eta}_{\mathcal{P}}$ and $\boldsymbol{\eta} \rightarrow \boldsymbol{\eta}_{\mathcal{E}}$ are linear in the e -parametrisation (X, \mathcal{P}) and (X, \mathcal{E}) are e -flat with respect to the induced metric D_{ψ} . Let $\boldsymbol{\mu}_{\mathcal{P}}$ be the expectation parameters of (X, \mathcal{P}) and $\boldsymbol{\mu}_{\mathcal{E}} = (\mu_s(\mathbf{v}, \mathbf{h})_{v,h})^T$ expectation coefficients (X, \mathcal{E}) , then the dual parametrisation $\boldsymbol{\mu}$ is given by:

$$\begin{aligned} \boldsymbol{\mu} &= \nabla \psi_{\mathcal{P}}(\boldsymbol{\eta}_{\mathcal{P}}) + \nabla \psi_{\mathcal{E}}(\boldsymbol{\eta}_{\mathcal{E}}) \\ &= (\boldsymbol{\mu}_{\mathcal{P}}, 0)^T + (0, \boldsymbol{\mu}_{\mathcal{E}})^T \\ &= (\boldsymbol{\mu}_{\mathcal{P}}, \boldsymbol{\mu}_{\mathcal{E}})^T \end{aligned}$$

Since the projections $\boldsymbol{\mu} \rightarrow \boldsymbol{\mu}_{\mathcal{P}}$ and $\boldsymbol{\mu} \rightarrow \boldsymbol{\mu}_{\mathcal{E}}$ are linear in the m -parametrisation (X, \mathcal{P}) and (X, \mathcal{E}) are m -flat with respect to the induced metric D_{ψ} . Therefore $(X, \mathcal{P}, D_{\psi})$ and $(X, \mathcal{E}, D_{\psi})$ are a dually flat submanifolds of $(X, \mathcal{U}, D_{\psi})$. □

8. MAXIMUM LIKELIHOOD ESTIMATION IN EXPONENTIAL FAMILIES WITH LATENT VARIABLES

Due to the existence of a simply connected embedding space $(X, \mathcal{U}, D_{\varphi})$ that covers (X, \mathcal{P}) as well as (X, \mathcal{E}) , also arbitrary smooth submanifolds (X, \mathcal{Q}) of (X, \mathcal{P}) may be connected to submanifolds $(X, \mathcal{E}_{\boldsymbol{\sigma}})$ of (X, \mathcal{E}) , given by a repeated observation $\boldsymbol{\sigma}$. Since $(X, \mathcal{U}, D_{\varphi})$ is furthermore a Riemannian statistical manifold and (X, \mathcal{Q}) and $(X, \mathcal{E}_{\boldsymbol{\sigma}})$ are smooth submanifolds of $(X, \mathcal{U}, D_{\varphi})$ geodesics between (X, \mathcal{Q}) and $(X, \mathcal{E}_{\boldsymbol{\sigma}})$ are given by the induced Riemannian metric D_{φ} .

Theorem 23. *Let (X, \mathcal{P}) be an exponential family over a partially observable measurable space (X, Σ) and (X, \mathcal{E}) an absolutely continuous empirical model over (X, Σ) . Let further be (X, \mathcal{Q}) a smooth submanifold of (X, \mathcal{P}) , and $\boldsymbol{\sigma}$ a repeated observation in (X, Σ) . Then a maximum likelihood estimation*

of (X, \mathcal{Q}) respective to σ is given by a minimal geodesic projection of (X, \mathcal{E}_σ) to (X, \mathcal{Q}) .

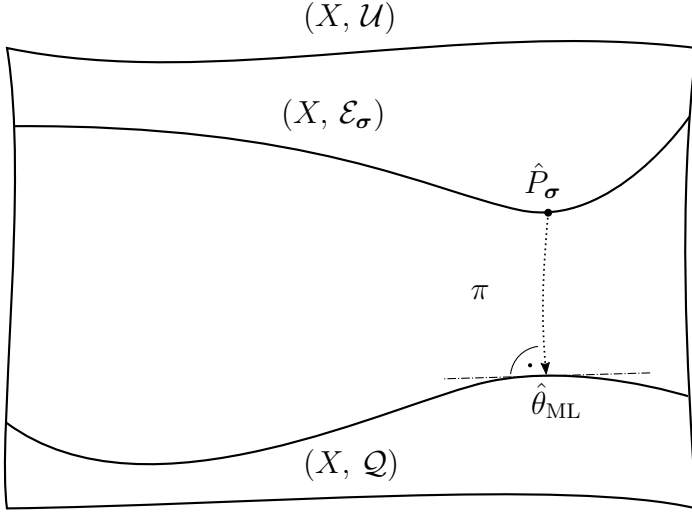


FIGURE 8.1. ML estimation in latent variable Exponential Families

Proof. Since (X, \mathcal{P}) is an exponential family and (X, \mathcal{E}) a continuous empirical model, there exists a common dually flat embedding space $(X, \mathcal{U}_\eta, D_\psi)$, such that (X, \mathcal{P}) and (X, \mathcal{E}) are dually flat submanifolds, with respect to the Bregman divergence D_ψ . Since the maximum likelihood estimation of \mathcal{Q} with respect to the repeated observation σ is independent of its chosen parametrisation, it may be obtained by the natural parametrisation of the embedding space $(X, \mathcal{U}_\eta, D_\psi)$, such that:

$$\hat{\theta}_{ML} \in \arg \max_{\eta} L[Q_\eta | \sigma]$$

Then theorem has an equivalent formulation, given by:

$$(8.1) \quad \arg \max_{\eta} L[Q_\eta | \sigma] = \arg \min_{\eta} d(P_\eta, Q_\eta)$$

Since (X, \mathcal{Q}) is a smooth submanifold of (X, \mathcal{P}) and (X, \mathcal{P}) of (X, \mathcal{U}) it follows, that (X, \mathcal{Q}) is also a smooth submanifold of (X, \mathcal{U}) and since (X, \mathcal{U}, D_ψ) is a dually flat statistical manifold, the projection theorem is satisfied. Therefore the geodesic projection $\pi : \mathcal{E}_\sigma \rightarrow \mathcal{Q}$ of a fixed point $P \in \mathcal{E}_\sigma$

to \mathcal{Q} is given by the minimal dual affine projection, and thus by a point $Q_\eta \in \mathcal{Q}$, that minimizes $D_\psi[Q_\eta || P]$, such that:

$$\arg \min_{\eta} d(P, Q_\eta) = \arg \min_{\eta} D_\psi[Q_\eta || P]$$

Then the minimal geodesic projection of \mathcal{E}_σ to \mathcal{Q} is given by points $P_\eta \in \mathcal{E}_\sigma$ and $Q_\eta \in \mathcal{Q}$, that minimize $D_\psi[Q_\eta || P_\eta]$:

$$(8.2) \quad \arg \min_{\eta} d(P_\eta, Q_\eta) = \arg \min_{\eta} D_\psi[Q_\eta || P_\eta]$$

Since η is the natural parametrisation of the exponential family (X, \mathcal{U}) , the Bregman divergence D_ψ is given by the dual Kullback-Leibler divergence in natural parameters. Therefore it follows, that:

$$(8.3) \quad \arg \min_{\eta} D_\psi[Q_\eta || P_\eta] = \arg \min_{\eta} D_{KL}[P_\eta || Q_\eta]$$

Without loss of generality let $\mathbf{v} : (X_v, \Sigma_v) \rightarrow V$ be the vectorial observable random variable and $\mathbf{h} : (X_h, \Sigma_h) \rightarrow H$ the vectorial latent random variable. Then $d\mathbf{v}$ and $d\mathbf{h}$ denote the Lebesgue measures in V and H and:

$$\begin{aligned} D_{KL}[P_\eta || Q_\eta] &= \int_X p_\eta(\mathbf{x}) \log \frac{p_\eta(\mathbf{x})}{q_\eta(\mathbf{x})} d\mathbf{x} \\ &= \int_{H, \sigma} p_\eta(\mathbf{v}, \mathbf{h}) \log \frac{p_\eta(\mathbf{v}, \mathbf{h})}{q_\eta(\mathbf{v}, \mathbf{h})} d\mathbf{v} d\mathbf{h} \end{aligned}$$

The common empirical distributions $p_\eta(\mathbf{v}, \mathbf{h})$ are defined by the marginal empirical densities $p_\eta(\mathbf{v})$ of the observable variables and conditional transition probabilities $p_\eta(\mathbf{h} | \mathbf{v})$ of the latent variables by $p_\eta(\mathbf{v}, \mathbf{h}) = p_\eta(\mathbf{v})p_\eta(\mathbf{h} | \mathbf{v})$, such that:

$$\begin{aligned} &D_{KL}[P_\eta || Q_\eta] \\ &= \int_{H, \sigma} p_\eta(\mathbf{v})p_\eta(\mathbf{h} | \mathbf{v}) \log \frac{p_\eta(\mathbf{v})p_\eta(\mathbf{h} | \mathbf{v})}{q_\eta(\mathbf{v}, \mathbf{h})} d\mathbf{v} d\mathbf{h} \end{aligned}$$

Furthermore the log function allows to write the product into a sum and to substitute the addends by functionals, such that:

$$\begin{aligned} &D_{KL}[P_\eta || Q_\eta] \\ &= F_1(P_\eta, Q_\eta) + F_2(P_\eta, Q_\eta) + F_3(P_\eta, Q_\eta) \end{aligned}$$

With:

$$\begin{aligned}
F_1(P_\eta, Q_\eta) &:= \int_{H, \sigma} p_\eta(\mathbf{v}) p_\eta(\mathbf{h} | \mathbf{v}) \log p_\eta(\mathbf{v}) d\mathbf{v} d\mathbf{h} \\
F_2(P_\eta, Q_\eta) &:= \int_{H, \sigma} p_\eta(\mathbf{v}) p_\eta(\mathbf{h} | \mathbf{v}) \log p_\eta(\mathbf{h} | \mathbf{v}) d\mathbf{v} d\mathbf{h} \\
F_3(P_\eta, Q_\eta) &:= - \int_{H, \sigma} p_\eta(\mathbf{v}) p_\eta(\mathbf{h} | \mathbf{v}) \log q_\eta(\mathbf{v}, \mathbf{h}) d\mathbf{v} d\mathbf{h}
\end{aligned}$$

Then it follows, that:

$$\begin{aligned}
F_1(P_\eta, Q_\eta) &= \int_{\sigma} p_\eta(\mathbf{v}) \log p_\eta(\mathbf{v}) \left(\int_H p_\eta(\mathbf{h} | \mathbf{v}) d\mathbf{h} \right) d\mathbf{v} \\
&= \int_{\sigma} p_\eta(\mathbf{v}) \log p_\eta(\mathbf{v}) d\mathbf{v} \\
&= -H[P_\eta | \sigma]
\end{aligned}$$

And furthermore::

$$\begin{aligned}
F_2(P_\eta, Q_\eta) &= \int_{\sigma} p_\eta(\mathbf{v}) \left(\int_H p_\eta(\mathbf{h} | \mathbf{v}) \log p_\eta(\mathbf{h} | \mathbf{v}) d\mathbf{h} \right) d\mathbf{v} \\
&= - \int_{\sigma} p_\eta(\mathbf{v}) H[p(\mathbf{h} | \mathbf{v}) | H] d\mathbf{v} \\
&= -H[p(\mathbf{h} | \mathbf{v}) | (H, \sigma)]
\end{aligned}$$

Then F_1 and F_2 are completely determined by σ , such that their minima do not depend on the choice of P_η and Q_η . Therefore:

$$\begin{aligned}
(8.4) \quad \arg \min_{\eta} D_{\text{KL}}[P_\eta \| Q_\eta] &= \arg \min_{\eta} F_3(P_\eta, Q_\eta) \\
&= \arg \max_{\eta} \int_{H, \sigma} p_\eta(\mathbf{v}) p_\eta(\mathbf{h} | \mathbf{v}) \log q_\eta(\mathbf{v}, \mathbf{h}) d\mathbf{v} d\mathbf{h} \\
&= \arg \max_{\eta} \int_X p_\eta(x) \log q_\eta(x) d\mu(x)
\end{aligned}$$

Since $p_\eta(x)$ are the empirical probabilities over (X, Σ) the conditions of lemma , equation 5.2, are satisfied, such that

$$\begin{aligned}
&\arg \max_{\eta} L[Q_\eta | \sigma] \\
&= \arg \max_{\eta} \int_X p_\eta(x) \log q_\eta(x) d\mu(x) \\
&\stackrel{8.4}{=} \arg \min_{\eta} D_{\text{KL}}[P_\eta \| Q_\eta] \\
&\stackrel{8.3}{=} \arg \min_{\eta} D_\psi[Q_\eta \| P_\eta] \\
&\stackrel{8.2}{=} \arg \min_{\eta} d(P_\eta, Q_\eta)
\end{aligned}$$

□

9. ALTERNATING MINIMIZATION

Let (X, \mathcal{P}, D_ψ) be a dually flat statistical manifold and (X, \mathcal{Q}) and (X, \mathcal{E}) smooth submanifolds of (X, \mathcal{P}, D_ψ) . Then the divergence D_ψ between (X, \mathcal{Q}) to (X, \mathcal{E}) is defined by the minimal divergence of its respective points, such that:

$$D_\psi[\mathcal{Q} \| \mathcal{S}] = \min_{Q \in \mathcal{Q}, S \in \mathcal{S}} D_\psi[Q \| S] = D_\psi[\hat{Q} \| \hat{S}]$$

where $\hat{Q} \in \mathcal{Q}$ and $\hat{S} \in \mathcal{S}$ minimize $D_\psi[Q \| S]$. By applying Amari's projection theorem it follows, that the pair (\hat{Q}, \hat{S}) also minimizes the geodesic distance and therefore has to be regarded as a pair of closest points between (X, \mathcal{Q}) and (X, \mathcal{S}) . Furthermore the dually flat structure allows an iterative alternating geodesic projection between (X, \mathcal{Q}) and (X, \mathcal{S}) to asymptotically approximate \hat{Q} and \hat{S} . This is termed alternating minimization.

Definition 24 (*Alternating minimization*). Let (X, \mathcal{U}) be an exponential family with smooth submanifolds (X, \mathcal{Q}) and (X, \mathcal{S}) . Then the alternating minimization from \mathcal{S} to \mathcal{Q} iteratively defines a sequence $(Q_n, S_n)_{n \in \mathbb{N}_0}$ of elements in $(\mathcal{Q}, \mathcal{S})$, which is given by:

Begin:

Let $S_0 \in \mathcal{S}$ be arbitrary

Iteration:

(m -step) Q_n is given by a geodesic projection of S_n to \mathcal{Q} :

$$Q_n = \pi(Q_n) = \arg \min_{Q \in \mathcal{Q}} d(S_n, Q)$$

(e -step) S_{n+1} is given by a dual geodesic projection of Q_n to \mathcal{S} :

$$S_{n+1} = \pi^*(Q_n) = \arg \min_{S \in \mathcal{S}} d(S, Q_n)$$

Theorem 25 (*Alternating minimization*). *Let (X, \mathcal{U}) be an exponential family model with smooth submanifolds (X, \mathcal{Q}) and (X, \mathcal{S}) . Then the alternating minimization algorithm converges in a pair of probability distributions, that locally minimize the geodesic distance between (X, \mathcal{Q}) and (X, \mathcal{S}) .*

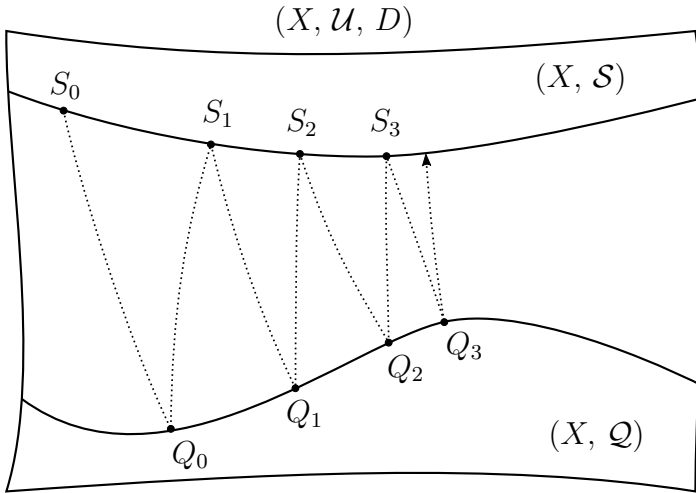


FIGURE 9.1. Alternating minimization in Exponential Families

Proof. Let (X, \mathcal{U}) be an exponential family, then the Bregman divergence of its cumulative generating function ψ induces a Riemannian metric and (X, \mathcal{U}, D_ψ) is a simply connected dually flat statistical manifold. Then (X, \mathcal{Q}, D_ψ) and (X, \mathcal{S}, D_ψ) are Riemannian submanifolds of (X, \mathcal{U}, D_ψ) , with respect to the induced Riemannian metric. In the m -step, the geodesic projection $\pi : \mathcal{S} \rightarrow \mathcal{Q}$ is given by the dual affine projection in the m -parametrisation

Then the dual affine projection minimizes the Bregman divergence and the Pythagorean theorem yields:

$$\begin{aligned} (9.1) \quad d(Q_n, S_n) &= D_\psi[S_n \parallel \pi(S_n)] \\ &\leq D_\psi[S_n \parallel \pi(S_n)] + D_\psi[\pi(S_n) \parallel R] \\ &= D_\psi[S_n \parallel Q_{n-1}] = d(Q_{n-1}, S_n) \end{aligned}$$

In the e -step dual geodesic projection $\pi^* : \mathcal{Q} \rightarrow \mathcal{S}$ is given by the affine projection in the e -parametrisation. Then the affine projection minimizes the dual Bregman divergence and the Pythagorean theorem yields:

$$\begin{aligned} (9.2) \quad d(Q_n, S_{n+1}) &= D_{\psi^*}[\pi(Q_n) \parallel Q_n] \\ &\leq D_{\psi^*}[R \parallel \pi(Q_n)] + D_{\psi^*}[\pi(Q_n) \parallel Q_n] \\ &= D_{\psi^*}[S_n \parallel Q_n] = d(Q_n, S_n) \end{aligned}$$

This proves, that $d(Q_n, S_n)$ monotonously decreases, since:

$$\begin{aligned} d(Q_{n+1}, S_{n+1}) &\stackrel{9.2}{\leq} d(Q_n, S_{n+1}) \\ &\stackrel{9.1}{\leq} d(Q_n, S_n), \forall n \in \mathbb{N}_0 \end{aligned}$$

Furthermore $d(Q_n, S_n)$ is bounded below by:

$$d(Q_n, S_n) = D_\psi[S_n \parallel S_n] \geq 0, \forall n \in \mathbb{N}_0$$

This proves, that $d(Q_n, S_n)$ converges against a local minimum. \square

Corollary 26. *Let (X, \mathcal{U}) be an exponential family with an e -flat submanifold (X, \mathcal{Q}) and an m -flat submanifold (X, \mathcal{S}) . Then the alternating minimization algorithm from \mathcal{S} to \mathcal{Q} converges against points, that globally minimize the geodesic distance between (X, \mathcal{Q}) and (X, \mathcal{S}) .*

Proof. Let $(Q_n, S_n)_{n \in \mathbb{N}_0}$ be a sequence, given by the alternating minimization algorithm from \mathcal{S} to \mathcal{Q} , then due to theorem 25 (Q_n, S_n) converges against points, that locally minimize the geodesic

distance between (X, \mathcal{Q}) and (X, \mathcal{S}) . Since (X, \mathcal{Q}) is e -flat and (X, \mathcal{S}) is m -flat corollary ?? is satisfied, such that this geodesic distance is unique and therefore (Q_n, S_n) converges against points, that globally minimize the geodesic distance between (X, \mathcal{Q}) and (X, \mathcal{S}) . \square

Corollary 27. *Let (X, \mathcal{P}) be an exponential family over a partially observable measurable space (X, Σ) and (X, \mathcal{E}) an absolutely continuous empirical model over (X, Σ) . Let further be (X, \mathcal{Q}) an e -flat submanifold of (X, \mathcal{P}) , and σ a repeated observation over (X, Σ) . Then a maximum likelihood estimation of (X, \mathcal{Q}) respective to σ is given by the limit of alternating minimization algorithm from \mathcal{E}_σ to \mathcal{Q} .*

Proof. Since (X, \mathcal{P}) is an exponential family and (X, \mathcal{E}) an absolutely continuous empirical model, there exists a common dually flat embedding space $(X, \mathcal{U}_\eta, D_\psi)$, such that (X, \mathcal{P}) and (X, \mathcal{E}) are dually flat submanifolds, with respect to the Bregman divergence D_ψ . Then (X, \mathcal{E}_σ) is m -flat in $(X, \mathcal{U}_\eta, D_\psi)$ and by definition (X, \mathcal{Q}) is e -flat in (X, \mathcal{P}) and therefore also in $(X, \mathcal{U}_\eta, D_\psi)$. This allows the application of corollary 26. \square