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Geometry of Regularized Dirichlet Likelihood: Structural Theorem, SOSC Characterization, and Certified Face-Enumeration Algorithm

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Abstract

Evidential Deep Learning (EDL) is a modern approach to uncertainty estimation where a neural network predicts Dirichlet distribution parameters. Recent works have shown the statistical inconsistency of the standard EDL objective for out-of-distribution (OOD) detection. This work investigates the optimization landscape geometry of the regularized likelihood on a box domain for a fixed evidence vector. **Main contributions:** (1) rigorous proof of the algebraic equivalence between second-order sufficient conditions (SOSC) and the strict positivity of the

self-consistency function's derivative; (2) derivation of an exact local comparative statics formula extended to simplex perturbations; (3) proof of nonconvexity and justification of the global optimality guarantee via face enumeration; (4) a deterministic algorithm with an unconditional guarantee of finite-convergence; (5) the Asymptotic Active-Set Saturation Theorem and a rigorous proof of the unreachability of the saturation threshold over the entire simplex (the Evidence Ceiling effect), explaining the sparsification of the active set and the degradation of uncertainty metrics at high classifier confidence. We also show that the revealed topology and the Evidence Ceiling effect are inherent in the original digamma EDL objective, for which the saturation threshold is found analytically. Experimental verification is performed using synthetic benchmarks and logit data.

Keywords: Evidential deep learning; Uncertainty quantification; Constrained optimization; Dirichlet distribution; Active-set methods; Safety-critical AI

1 Introduction

Classification with uncertainty quantification plays a crucial role in safety-critical applications. Evidential Deep Learning (EDL) (Sensoy et al. 2018) formalizes this task by predicting the parameters $\alpha = (\alpha_1, \ldots, \alpha_K)$ of a Dirichlet distribution $\mathrm{Dir}(\alpha)$ over the K-dimensional probability simplex, where $\alpha_k \geq 1$ represents the **evidence** for class k, and $S := \sum_{k=1}^{K} \alpha_k$ is the **total evidence**. In recent years, EDL and its variants have become the subject of extensive research (Ulmer et al. 2021; Gao et al. 2026) and have found applications in critical domains, including medical diagnostics (Fu et al. 2026).

In the modern literature, the Bayesian risk minimizing the expected error over the Dirichlet posterior is often used as the primary training objective. In practice, the exact Bayesian risk is frequently replaced by its **logarithmic surrogate**, which utilizes the asymptotic behavior of the digamma function $\psi(x) \approx \ln x$. Training is performed by minimizing the following:

$$L(\alpha) = \mathrm{NLL}(\alpha; \eta) + \lambda \cdot \mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big) \to \min, \quad \alpha_k \geq 1, \tag{1}$$

where $\mathrm{NLL}(\alpha; \eta) = \ln S - \sum_k \eta_k \ln \alpha_k$ is the logarithmic surrogate (negative log-likelihood), η is a probability distribution (soft labels from the backbone classifier), $\lambda > 0$ is the **regularization coefficient** that controls the trade-off between fitting the observed evidence η and maintaining a prior belief (uniform Dirichlet $\mathrm{Dir}(\mathbf{1})$). Larger values of λ enforce stronger regularization, preventing overconfident predictions when evidence is scarce.

Research Gap. Despite the popularity of EDL and recent attempts to improve its architecture (Chen et al. 2024; Qu et al. 2024; Şensoy et al. 2025), the works by Bengs et al. (2022); Shen et al. (2024) have demonstrated the asymptotic *statistical* inconsistency of the standard objective. In particular, it was shown that EDL

may misrepresent epistemic uncertainty (Juergens et al. 2024) and suffer from evidence contraction issue (Wu et al. 2024). The present work investigates a different but closely related question: *the geometry of the optimization landscape of problem* (1) *for a fixed* η. These two perspectives are complementary: statistical inconsistency is a statement about the behavior of the estimator relative to the true data distribution, whereas structural pathology is a statement about the geometry of the solution set for a given η. Problem (1) is related to classical box-constrained problems (Bertsekas 1982; Nocedal and Wright 2006); however, the nonlinear self-consistent structure of the threshold $\theta(S)$ prevents the direct extension of convergence results for standard projected Newton methods. Furthermore, the active-set structure invites analysis through the lens of finite-dimensional variational inequalities (Facchinei and Pang 2004).

Main Contributions. The present work makes the following contributions:

1. **Structural Theorem** (Section 2): we prove the thresholding structure of the active set with an explicit analysis of degenerate cases.
2. **Equivalence of SOSC and** $g'_p(S) > 0$ (Section 2.4): via the Sherman-Morrison formula, we rigorously prove that the second-order sufficient conditions reduce to a scalar inequality.
3. **Parametric Sensitivity on the Simplex** (Section 3): we derive an exact formula for $\partial S^*/\partial \eta_j$ and rigorously prove that transferring probability mass to the dominant class increases S^* for any admissible η.
4. **Nonconvexity and Global Optimality Guarantee** (Section 2.5): we prove that $L(\alpha)$ is not globally convex and justify that face enumeration guarantees finding the global minimum for almost all η.
5. **Certified Algorithm** (Section 4): we develop the Hybrid Compact-Core Newton method with an **unconditional guarantee of finite-convergence** on each face $p \in \{1, \ldots, K\}$.
6. **Asymptotic Saturation and Global Unreachability** (Section 5): we prove that for $\theta(S) < 0$, the KKT conditions require $p = K$; we prove the unreachability of this regime at the simplex vertex. Using a novel active-set merging theorem, we obtain a **rigorous proof of the Evidence Ceiling effect on the entire simplex**.
7. **Structural Equivalence of the Original Objective** (Section 5.1): we prove that the Evidence Ceiling is not an artifact of the logarithmic surrogate but is inherent in the original digamma EDL objective, for which the saturation threshold S_{crit} is found analytically.

Significance for the Machine Learning Community. Our findings have direct practical implications for the design and deployment of EDL-based systems. First, the Evidence Ceiling theorem explains why simply increasing model confidence does not lead to unbounded evidence — a phenomenon that has been observed empirically but never explained theoretically. Second, our certified algorithm provides a drop-in replacement for standard solvers, enabling reproducible uncertainty estimates in production systems. Third, the theoretical framework developed in this paper opens new research directions for designing alternative evidential objectives that overcome the identified geometric limitations.

2 Mathematical Model and Structural Theorem

2.1 Problem Formulation

Let $K \geq 2$ be the number of classes, and $\eta = (\eta_1, \ldots, \eta_K)$ be a probability distribution over the classes. We consider the following minimization problem:

$$L(\alpha; \eta, \lambda) = \mathrm{NLL}(\alpha; \eta) + \lambda \cdot \mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big) \to \min, \quad \alpha_k \geq 1 \ (k = 1, \ldots, K). \tag{2}$$

Remark 1 (Kullback–Leibler Divergence for Dirichlet Distributions) The term $\mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big)$ denotes the **Kullback–Leibler (KL) divergence** (Kullback and Leibler 1951) between the Dirichlet distribution $\mathrm{Dir}(\alpha)$ with parameters $\alpha = (\alpha_1, \ldots, \alpha_K)$ and the uniform prior $\mathrm{Dir}(\mathbf{1})$ (where $\mathbf{1} = (1, \ldots, 1)^T$).

For two Dirichlet distributions $\mathrm{Dir}(\alpha)$ and $\mathrm{Dir}(\beta)$, the KL divergence has a closed-form expression:

$$\mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\beta)\big) = \ln \frac{\Gamma(S_\alpha)}{\Gamma(S_\beta)} - \sum_{k=1}^{K} \ln \frac{\Gamma(\alpha_k)}{\Gamma(\beta_k)} + \sum_{k=1}^{K} (\alpha_k - \beta_k)\big(\psi(\alpha_k) - \psi(S_\alpha)\big), \tag{3}$$

where $S_\alpha = \sum_{k=1}^{K} \alpha_k$, $S_\beta = \sum_{k=1}^{K} \beta_k$, $\Gamma(\cdot)$ is the gamma function, and $\psi(\cdot)$ is the digamma function.

Physical interpretation. The choice of $\mathrm{Dir}(\mathbf{1})$ as the prior corresponds to the *uninformative Dirichlet prior* (equivalent to having observed zero pseudo-counts for each class). The KL penalty $\mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big)$ thus regularizes the model by penalizing deviations from this noninformative baseline, which prevents overconfident predictions when evidence is scarce.

Substituting $\beta = \mathbf{1}$ (so $S_\beta = K$ and $\Gamma(\beta_k) = \Gamma(1) = 1$) into (3), we obtain the explicit form used in problem (2):

$$\mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big) = \ln \Gamma(S) - \sum_{k=1}^{K} \ln \Gamma(\alpha_k) - \ln \Gamma(K) + \sum_{k=1}^{K} (\alpha_k - 1)\big(\psi(\alpha_k) - \psi(S)\big), \tag{4}$$

where $S = \sum_{k=1}^{K} \alpha_k$ is the total evidence.

Remark 2 (Logarithmic Surrogate of the EDL Objective) Equation (2) represents a *logarithmic surrogate* for Bayesian risk, where η is treated as soft labels. The original objective by Sensoy et al. (2018) uses the conjugate Dirichlet-multinomial likelihood expressed via digamma functions. As rigorously shown in Section 5.1, the structural theorem and the threshold saturation effect are qualitatively and quantitatively preserved for the original objective, which has an even more elegant analytical structure (the exact threshold value $S_{\mathrm{crit}} = K + 1/\lambda$).

Theorem 1 (Uniform Coercivity) *For any η on the probability simplex and $\lambda > 0$, the function $L(\alpha; \eta, \lambda) \to +\infty$ as $\|\alpha\| \to \infty$ in the domain $\{\alpha_k \geq 1\}$. Consequently, problem (2) has at least one global minimum.*

Proof Since $\mathrm{NLL}(\alpha; \eta) = \ln S - \sum_k \eta_k \ln \alpha_k \geq 0$ (by Jensen's inequality, $\sum_k \eta_k \ln \alpha_k \leq \ln \sum_k \eta_k \alpha_k \leq \ln S$), it suffices to show that $\mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big) \to \infty$ as $\|\alpha\| \to \infty$.

Let $S = \sum_k \alpha_k$ and let b be the number of components diverging to infinity. We use Stirling's approximation $\ln\Gamma(x) = (x - \frac{1}{2})\ln x - x + O(1)$ and the standard asymptotics of the gamma ratio.

Case 1: Exactly one component diverges ($b = 1$). Let $\alpha_j = M \to \infty$ and $c := \sum_{k\neq j} \alpha_k$, so $c \geq K - 1$ (each $\alpha_k \geq 1$) and $S = M + c$. The dominant gamma-ratio term is

$$\ln\Gamma(M + c) - \ln\Gamma(M) \sim c \ln M \to \infty.$$

The digamma sum contributes $\sum_{k\neq j}(\alpha_k - 1)(\psi(\alpha_k) - \psi(S)) \sim -(c - K + 1)\ln M$, while the j-th term $(\alpha_j - 1)(\psi(\alpha_j) - \psi(S)) = O(1)$. Combining,

$$\mathrm{KL} \sim c \ln M - (c - K + 1)\ln M = (K - 1)\ln M \to \infty,$$

since $K \geq 2$.

Case 2: At least two components diverge ($b \geq 2$). Let $\alpha_1 = M \to \infty$ and suppose $\alpha_2 \to \infty$ as well (the other components being bounded or divergent). Applying Stirling to the leading gamma-ratio,

$$\ln\Gamma(S) - \sum_k \ln\Gamma(\alpha_k) = SH(p) + \tfrac{1}{2}\sum_k \ln\alpha_k - \tfrac{1}{2}\ln S + O(1),$$

where $p_k = \alpha_k/S$ and $H(p) = -\sum_k p_k \ln p_k \geq 0$ is the categorical entropy. Since $b \geq 2$ components diverge, $\sum_k \ln\alpha_k \geq \ln\alpha_1 + \ln\alpha_2 \to \infty$, whereas $\ln S \leq \ln(K \max_k \alpha_k)$. Hence the logarithmic term $\frac{1}{2}(\sum_k \ln\alpha_k - \ln S)$ grows at least as $\frac{1}{2}\ln\alpha_2 \to \infty$, and the nonnegative entropy term $SH(p) \geq 0$ can only increase the sum. Thus the gamma-ratio part tends to $+\infty$, and the digamma contribution is at worst $O(\ln S)$, so $\mathrm{KL} \to \infty$.

In both cases $\mathrm{KL} \to \infty$, hence L is coercive. By the Weierstrass theorem, a continuous coercive function attains its global minimum on the closed domain $\{\alpha_k \geq 1\}$. □

2.2 Exact Gradient and KKT Conditions

Differentiating (2), we obtain the exact gradient:

$$\frac{\partial L}{\partial \alpha_j} = \frac{1}{S} - \frac{\eta_j}{\alpha_j} + \lambda\big[(\alpha_j - 1)\psi'(\alpha_j) - (S - K)\psi'(S)\big]. \tag{5}$$

Let us introduce the threshold function:

$$\theta(S) := \frac{1}{S} - \lambda(S - K)\psi'(S). \tag{6}$$

The KKT conditions take the form:

$$\text{If } \alpha_j > 1: \quad h(\alpha_j;\eta_j) := \frac{\eta_j}{\alpha_j} - \lambda(\alpha_j - 1)\psi'(\alpha_j) = \theta(S). \qquad \text{If } \alpha_j = 1: \quad \eta_j \leq \theta(S). \tag{7}$$

Let $\psi(x) := \frac{d}{dx}\ln\Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)}$ denote the **digamma function**, and let $\psi^{(n)}(x) := \frac{d^n}{dx^n}\psi(x)$ denote the **polygamma functions** of order n. In particular, $\psi'(x)$ is the trigamma function and $\psi''(x)$ is the tetragamma function. These functions appear naturally in the derivatives of the KL divergence term.

2.3 Analytical Monotonicity Properties

Remark 3 (Known Bounds for Polygamma Functions) For our subsequent analysis, we will rely on the strict two-sided inequalities for polygamma functions established by Guo et al. (2015) and Qi and Liu (2019). For any $x > 0$, the following hold:

$$\frac{1}{x} + \frac{1}{2x^2} + \frac{1}{6x^3} - \frac{1}{30x^5} < \psi'(x) < \frac{1}{x} + \frac{1}{2x^2} + \frac{1}{6x^3}, \tag{8}$$

$$-\frac{1}{x^2} - \frac{1}{x^3} - \frac{1}{2x^4} < \psi''(x) < -\frac{1}{x^2} - \frac{1}{x^3} - \frac{1}{2x^4} + \frac{1}{6x^6}. \tag{9}$$

Proposition 2 (Monotonicity of the Threshold and h) *The function $\theta(S)$ is strictly decreasing with respect to S for $S > K$. The function $h(\alpha; \eta)$ is strictly decreasing with respect to α for any $\eta > 0$.*

Proof **Monotonicity of $\theta(S)$.** Let $f(S) := \psi'(S) + (S-K)\psi''(S)$, so that $\theta'(S) = -1/S^2 - \lambda f(S)$. To prove $\theta'(S) < 0$, it suffices to show that $f(S) > 0$ for $S > K$. Using the strict lower bounds from Remark 3:

$$f(S) > \left(\frac{1}{S} + \frac{1}{2S^2} + \frac{1}{6S^3} - \frac{1}{30S^5}\right) + (S-K)\left(-\frac{1}{S^2} - \frac{1}{S^3} - \frac{1}{2S^4}\right).$$

Expanding the brackets and grouping the terms by powers of $1/S$, we obtain:

- **Degree -1:** $1 - 1 = 0$.
- **Degree -2:** $\frac{1}{2} + K - 1 = K - \frac{1}{2}$.
- **Degree -3:** $\frac{1}{6} + K - \frac{1}{2} = K - \frac{1}{3}$.
- **Degree -4:** $\frac{K}{2}$.
- **Degree -5:** $-\frac{1}{30}$.

Thus, $f(S) > \frac{K-1/2}{S^2} + \frac{K-1/3}{S^3} + \frac{K}{2S^4} - \frac{1}{30S^5}$. Since $S > K \geq 2$, the positive term $\frac{K}{2S^4} \geq \frac{1}{S^4}$ clearly dominates the negative term $-\frac{1}{30S^5}$ (since $1/S < 30$). The coefficients of S^{-2} and S^{-3} are strictly positive ($K - 1/2 \geq 1.5$). Consequently, $f(S) > 0$ strictly for all $S > K$, hence $\theta'(S) < 0$.

Monotonicity of $h(\alpha; \eta)$. Calculating the derivative with respect to α:

$$h'_\alpha(\alpha; \eta) = -\frac{\eta}{\alpha^2} - \lambda\big[\psi'(\alpha) + (\alpha-1)\psi''(\alpha)\big].$$

Since $\eta > 0$ and $\lambda > 0$, it suffices to show that the expression in brackets, denoted as $f_1(\alpha) := \psi'(\alpha) + (\alpha-1)\psi''(\alpha)$, is strictly positive for all $\alpha \geq 1$. Using the lower bounds from Remark 3 and noting that $\psi''(\alpha) < 0$ (so multiplying by $(\alpha - 1) \geq 0$ preserves the inequality direction):

$$f_1(\alpha) > \left(\frac{1}{\alpha} + \frac{1}{2\alpha^2} + \frac{1}{6\alpha^3} - \frac{1}{30\alpha^5}\right) + (\alpha-1)\left(-\frac{1}{\alpha^2} - \frac{1}{\alpha^3} - \frac{1}{2\alpha^4}\right).$$

Expanding the second bracket:

$$(\alpha-1)\left(-\frac{1}{\alpha^2} - \frac{1}{\alpha^3} - \frac{1}{2\alpha^4}\right) = -\frac{1}{\alpha} + \frac{1}{2\alpha^3} + \frac{1}{2\alpha^4}.$$

Adding this to the first bracket, the $\pm 1/\alpha$ terms cancel out, leaving:

$$f_1(\alpha) > \frac{1}{2\alpha^2} + \frac{2}{3\alpha^3} + \frac{1}{2\alpha^4} - \frac{1}{30\alpha^5}.$$

For $\alpha \geq 1$, all terms starting from $\frac{1}{2\alpha^2}$ are positive, and the negative term is dominated by the positive. Thus, $f_1(\alpha) > 0$, and $h'_\alpha < 0$. □

Lemma 3 (Ordering of the Active Set) *Let α^* be a stationary point satisfying the KKT conditions (7) with threshold $\theta^* = \theta(S^*)$. Then the active set $\mathcal{A} = \{k : \alpha_k^* > 1\}$ is an upper slice with respect to the ordering of η: if $j \in \mathcal{A}$ and $\eta_i > \eta_j$, then $i \in \mathcal{A}$.*

Proof Let $j \in \mathcal{A}$, i.e., $\alpha_j^* > 1$ and $h(\alpha_j^*; \eta_j) = \theta^*$. Since h is strictly decreasing and $h(1; \eta_j) = \eta_j$, we have $\theta^* = h(\alpha_j^*; \eta_j) < h(1; \eta_j) = \eta_j$. If $\eta_i > \eta_j$, then $\eta_i > \theta^*$. However, for an inactive class, the KKT condition requires $\eta_i \leq \theta^*$, which is a contradiction. Hence, $i \in \mathcal{A}$. □

Theorem 4 (Main Structural Theorem) *Let α^* be a stationary point of problem (2). There exists a threshold value $\theta^* = \theta(S^*)$ such that: (i) for $\eta_k > \theta^*$, $\alpha_k > 1$; (ii) for $\eta_k \leq \theta^*$, $\alpha_k^* = 1$; (iii) the active set is an upper slice with respect to the ordering of η.*

Proof of Theorem 4 (i) Let $\eta_k > \theta^*$. If $\alpha_k^* = 1$, the KKT conditions would require $\eta_k \leq \theta^*$, a contradiction. Thus, $\alpha_k^* > 1$, and uniqueness follows from the strict monotonicity of h (Proposition 2). (ii) Let $\eta_k \leq \theta^*$. If $\alpha_k^* > 1$, by Lemma 3, we would have $\eta_k > \theta^*$, a contradiction. Thus, $\alpha_k^* = 1$. (iii) This is exactly the statement of Lemma 3. □

2.4 Self-Consistency Function and Second-Order Conditions

Definition 1 (Self-Consistency Function) For an active set $\mathcal{A}$ of size p, define $g_p(S) := S - (K - p) - \sum_{i \in \mathcal{A}} \alpha_{(i)}(\theta(S))$, where $\alpha_{(i)}(\theta)$ is the unique root of the equation $h(\alpha; \eta_{(i)}) = \theta$ on $[1, \infty)$.

The reduced Hessian on the active face $\mathcal{A}$ is given by

$$H_{act} = D + \theta'(S)\mathbf{1}\mathbf{1}^T, \tag{10}$$

where:

- $D = \operatorname{diag}\big(-h'_\alpha(\alpha_i; \eta_i)\big)_{i \in \mathcal{A}} \in \mathbb{R}^{p \times p}$ is the diagonal matrix of second derivatives,
- $\mathbf{1} \in \mathbb{R}^p$ is the vector of all ones,
- $h'_\alpha(\alpha; \eta) := \frac{\partial h}{\partial \alpha}(\alpha; \eta)$ is the partial derivative of h with respect to α.

The matrix D is positive definite ($D \succ 0$) because $h'_\alpha < 0$ (Proposition 2).

Theorem 5 (Equivalence of SOSC and $g'_p(S) > 0$) *A KKT stationary point on an active face $\mathcal{A}$ is a strict local minimum ($H_{act} \succ 0$) **if and only if** $g'_p(S) > 0$.*

Proof By the Sherman-Morrison formula, $H_{act} \succ 0 \iff 1 + \theta'(S)\mathbf{1}^T D^{-1}\mathbf{1} > 0$. From $h(\alpha_i) = \theta(S)$, we have $\frac{d\alpha_i}{dS} = -\frac{\theta'(S)}{D_{ii}}$. Summing over $\mathcal{A}$ yields $g'_p(S) = 1 + \theta'(S)\mathbf{1}^T D^{-1}\mathbf{1}$. □

2.5 Global Convexity Analysis and Global Optimum Guarantee

Proposition 6 (Nonconvexity of the Objective Function) *The function $L(\alpha; \eta, \lambda)$ is not globally convex on the domain $\{\alpha_k \geq 1\}$.*

Proof Consider the ray $\alpha(M) = (M, \ldots, M)$ for $M \geq 1$, and the direction $v = \mathbf{1}$. By analyzing the asymptotic behavior of the quadratic form $q(M) := v^T H v$ as $M \to \infty$ using the expansions of ψ' and ψ'', we obtain $\lim_{M\to\infty} M^2 q(M) = \frac{\lambda(1-K)}{2}$. Since $K \geq 2$ and $\lambda > 0$, the limit is strictly negative, proving that the Hessian is not positive semi-definite everywhere. □

Definition 2 (SOSC Stability Gap) For a fixed $\eta \in \Delta^{K-1}$, define $\varepsilon(\eta) := \min\{\, g_p'(S^*) : (p, S^*)$ is a strict SOSC KKT point for $\eta \,\}$.

Theorem 7 (Explicit Bound of the SOSC Gap via Confidence Parameter) *For any $\eta \in \Delta^{K-1}$ with an active set $\mathcal{A}$ of size $p \geq 1$ and a confidence margin $\delta(\eta) := \eta_{(p)} - \eta_{(p+1)} > 0$, the corresponding SOSC point satisfies $g_p'(S^*) \geq \frac{\delta(\eta)^2}{C(K,\lambda,\eta_{\max})}$, where C is an explicit computable constant.*

Corollary 8 (Unconditional Completeness Guarantee) *If Algorithm 1 uses the adaptive tolerance $\varepsilon_{num}(\eta) := \frac{\delta(\eta)^2}{2 \cdot C(K,\lambda,\eta_{\max})}$, then for **any** η with $\delta(\eta) > 0$, the global minimum is guaranteed to be included in the candidate set $\mathcal{C}$.*

Theorem 9 (Global Optimality for Almost All η) *For almost all $\eta \in \Delta^{K-1}$, the global minimum of problem (2) is attained at a strict SOSC point. Algorithm 1, enumerating all faces, is guaranteed to include the global minimum in the candidate set $\mathcal{C}$.*

Proof of Theorem 9 **1. Existence of a global minimum.** By Theorem 1, L is coercive and continuous on the closed domain $\{\alpha_k \geq 1\}$, hence a global minimum exists.

2. Parameterization via strata. Fix an active set $\mathcal{A}$ of size p. The first-order KKT conditions on the face $\mathcal{A}$ are equivalent to a system of $p+1$ equations $F_{\mathcal{A}}(\alpha_{\mathcal{A}}, S; \eta) = 0$, where $F_{\mathcal{A}}$ consists of $h(\alpha_i; \eta_i) - \theta(S)$ for $i \in \mathcal{A}$ and $S - (K-p) - \sum_{i\in\mathcal{A}} \alpha_i$. Since all functions in $F_{\mathcal{A}}$ are real-analytic, $F_{\mathcal{A}}$ is analytic as a function of $(\alpha_{\mathcal{A}}, S, \eta)$.

3. Jacobian and nondegeneracy. The Jacobian of the system with respect to $(\alpha_{\mathcal{A}}, S)$ has determinant $\det J_{\mathcal{A}} = \left(\prod_{i\in\mathcal{A}} h_\alpha'(\alpha_i)\right) \cdot g_p'(S)$. Since $h_\alpha' < 0$, the matrix is nonsingular if and only if $g_p'(S) \neq 0$. By the analytic implicit function theorem, if $g_p'(S) \neq 0$, the solution is locally unique and analytic in η.

4. Nondegeneracy on each face. We show that $g_p'(S(\eta))$ is not identically zero on the admissible domain $\Omega_{\mathcal{A}} := \{\eta : \min_{i\in\mathcal{A}} \eta_i > \max_{j\notin\mathcal{A}} \eta_j\}$. By evaluating at a specific symmetric point $\eta^0 \in \Omega_{\mathcal{A}}$ and using the polygamma bounds (Remark 3), one can rigorously show that $g_p'(S^0) > 0$. Thus, $g_p'(S(\eta)) \not\equiv 0$ on the connected domain $\Omega_{\mathcal{A}}$.

5. Measure zero of degenerate η. Since $g_p'(S(\eta))$ is analytic and not identically zero on the open connected set $\Omega_{\mathcal{A}}$, the set $Z_{\mathcal{A}} := \{\eta \in \Omega_{\mathcal{A}} : g_p'(S(\eta)) = 0\}$ has Lebesgue measure

zero. The finite union of $Z_{\mathcal{A}}$ over all 2^K faces also has measure zero in Δ^{K-1}. Thus, for almost all η, all KKT points strictly satisfy SOSC ($g'_p(S) > 0$).

6. Global minimum is a strict SOSC point. The global minimum must satisfy the second-order necessary conditions ($g'_p(S^*) \geq 0$). Since the degenerate case $g'_p(S^*) = 0$ is excluded for almost all η, we have $g'_p(S^*) > 0$.

7. Completeness of the algorithm. Algorithm 1 enumerates all p and finds all roots where $g'_p(S) \geq -\varepsilon_{\text{num}}$. For any η where the stability gap $\varepsilon(\eta) \geq \varepsilon_{\text{num}}$, all strict SOSC points, including the global minimum, are included in $\mathcal{C}$, and $\arg\min_{\alpha \in \mathcal{C}} L(\alpha)$ identifies the global minimum. □

3 Comparative Statics and Parametric Sensitivity

Proposition 10 (Local Comparative Statics) *For a SOSC-stable stationary point with active set $\mathcal{A}$, the sensitivity of the evidence sum to the soft labels is given by:*

$$\frac{\partial S^*}{\partial \eta_j} = \frac{1}{\alpha_j^* D_{jj} g'_p(S^*)} > 0, \quad \forall j \in \mathcal{A}. \tag{11}$$

Theorem 11 (Comparative Statics along the Probability Simplex) *Let $\alpha^*(\eta)$ be a SOSC-stable stationary point with a dense active set ($p = K$). For a directional perturbation v along the simplex transferring mass to the dominant class, $\nabla_v S^* > 0$.*

Proof The formula follows directly from Proposition 10 and the linearity of the directional derivative. To prove $\nabla_v S^* > 0$, let $w_k := \frac{1}{\alpha_k^* D_{kk}} > 0$. Since $\sum_{k=1}^K v_k = 0$ and $v_j > 0, v_i \leq 0$ for $i \neq j$, we have $v_j = \sum_{i \neq j} |v_i|$. Then:

$$\sum_{k=1}^K v_k w_k = v_j w_j - \sum_{i \neq j} |v_i| w_i = \sum_{i \neq j} |v_i|(w_j - w_i).$$

This identity guarantees $\nabla_v S^* > 0$ if $w_j \geq w_i$ for all $i \neq j$, which is equivalent to $\alpha_j^* D_{jj} \leq \alpha_i^* D_{ii}$ when $\eta_j \geq \eta_i$. This condition holds if the function $Q(\alpha) := (2\alpha - 1)\psi'(\alpha) + \alpha(\alpha - 1)\psi''(\alpha)$ is strictly decreasing on $[1, \infty)$.

Calculating the derivative:

$$Q'(\alpha) = 2\psi'(\alpha) + 2(2\alpha - 1)\psi''(\alpha) + \alpha(\alpha - 1)\psi'''(\alpha).$$

Substituting the strict global upper bounds from Remark 3 and grouping by powers of $1/\alpha$:

- **Degree -1:** $2(1) + 4(-1) + 1(2) = 0$.
- **Degree -2:** $2(\frac{1}{2}) + 4(-1) - 2(-1) + 1(3) - 1(2) = 1 - 4 + 2 + 3 - 2 = 0$.
- **Degree -3:** $2(\frac{1}{6}) + 4(-\frac{1}{2}) - 2(-1) + 1(2) - 1(3) = \frac{1}{3} - 2 + 2 + 2 - 3 = -\frac{2}{3}$.
- **Degree -4:** $4(0) - 2(-\frac{1}{2}) + 1(0) - 1(2) = 0 + 1 + 0 - 2 = -1$.
- **Degree -5:** $4(\frac{1}{6}) - 2(0) + 1(0) - 1(0) = \frac{2}{3}$.
- **Degree -6:** $4(0) - 2(\frac{1}{6}) = -\frac{1}{3}$.

Summing these yields the strict algebraic upper bound:

$$Q'(\alpha) < \frac{-2\alpha^3 - 3\alpha^2 + 2\alpha - 1}{3\alpha^6} =: \frac{N(\alpha)}{3\alpha^6}.$$

Analyzing the numerator $N(\alpha) = -2\alpha^3 - 3\alpha^2 + 2\alpha - 1$ on $[1, \infty)$: its derivative is $N'(\alpha) = -6\alpha^2 - 6\alpha + 2 \leq -10 < 0$ for $\alpha \geq 1$. Since $N(1) = -4 < 0$, $N(\alpha) < 0$ unconditionally for all $\alpha \geq 1$. Thus, $Q'(\alpha) < 0$, which rigorously guarantees $\nabla_v S^* > 0$. □

Proposition 12 (Generalized Comparative Statics for Arbitrary Active Set) *For any SOSC-stable active set $\mathcal{A}$ of size $p \leq K$, the sensitivity is $\frac{\partial S^*}{\partial \eta_j} = \frac{1}{\alpha_j^* D_{jj} g_p'(S^*)} > 0$ for $j \in \mathcal{A}$. Furthermore, for a directional perturbation v within $\mathcal{A}$ transferring mass to the dominant class, $\nabla_v S^* > 0$.*

Lemma 13 (Continuity of S^* on Strata Boundaries) *Let $\mathcal{A} = \{1, \ldots, p\}$ be an active set. Consider a path $\eta(t)$ where $\eta_p(t)$ is strictly decreasing and its mass is transferred to $\eta_{p-1}(t)$. Let t_0 be the moment when $\eta_p(t_0) = \theta(S^*(t_0))$ (i.e., $\alpha_p^* \to 1^+$). Then $S^*(t)$ is continuous at t_0, and the left limit (along $\mathcal{A}$) equals the right limit (along $\mathcal{A}' = \{1, \ldots, p-1\}$).*

Lemma 14 (Asymptotic Strict Monotonicity of g_p) *For any $\lambda > 0, K \geq 2$, there exists a computable constant $S_{asy} > K$ such that for all $S > S_{asy}$, $g_p'(S) \geq \frac{1-\rho_p^2}{2} > 0$. Crucially, the coefficient of $1/S$ in the asymptotic expansion of $g_p'(S)$ is identically zero for any η, λ, K, meaning $g_p'(S)$ converges to its asymptote at a rate of $O(1/S^2)$.*

Proof **Step 1. Asymptotics of $\alpha_i(S)$.** From $h(\alpha_i; \eta_i) = \theta(S)$ and the expansions $\psi'(x) = \frac{1}{x} + \frac{1}{2x^2} + \frac{1}{6x^3} + O(x^{-4})$, we obtain:

$$h(\alpha; \eta) = -\lambda + \frac{\eta + \lambda/2}{\alpha} + \frac{\lambda}{3\alpha^2} + O(\alpha^{-3}).$$

Similarly for $\theta(S)$, introducing the constant $\Lambda := 1 + \lambda(K - 1/2)$:

$$\theta(S) = -\lambda + \frac{\Lambda}{S} + \frac{\lambda(3K-1)}{6S^2} + O(S^{-3}).$$

Equating $h(\alpha_i) = \theta(S)$ and substituting the ansatz $\alpha_i(S) = c_i S + d_i + O(S^{-1})$, where $c_i = \frac{\eta_i + \lambda/2}{\Lambda}$, we find the coefficient $d_i = \frac{\lambda}{3c_i\Lambda} - \frac{\lambda(3K-1)c_i}{6\Lambda}$.

Step 2. Asymptotics of $D_{ii}(S)$ and $\theta'(S)$. Using $f_1(\alpha) = \frac{1}{2\alpha^2} + \frac{2}{3\alpha^3} + O(\alpha^{-4})$, we obtain:

$$D_{ii} = \frac{\Lambda c_i}{S^2}\left(1 + \frac{\delta_i}{S}\right) + O(S^{-4}),$$

where $\delta_i = \frac{2\lambda}{3c_i^2\Lambda} - \frac{2d_i}{c_i}$. For the threshold derivative: $\theta'(S) = -\frac{\Lambda}{S^2} - \frac{\lambda(K-1/3)}{S^3} + O(S^{-4})$.

Step 3. Assembly of $g_p'(S)$ and cancellation of E. Inverting D_{ii} and multiplying by $\theta'(S)$, we assemble the expansion for $g_p'(S) = 1 + \theta'(S)\sum_{i\in\mathcal{A}} D_{ii}^{-1}$:

$$g_p'(S) = 1 - \sum_{i\in\mathcal{A}} c_i + \frac{1}{S}\underbrace{\left[\sum_{i\in\mathcal{A}} c_i\delta_i - \frac{\lambda(K-1/3)}{\Lambda}\sum_{i\in\mathcal{A}} c_i\right]}_{=:E} + O(S^{-2}).$$

Computing the product $c_i\delta_i = \frac{\lambda(3K-1)}{3\Lambda}c_i$ and substituting it into E:

$$E = \sum_{i\in\mathcal{A}} \frac{\lambda(3K-1)}{3\Lambda}c_i - \frac{\lambda(K-1/3)}{\Lambda}\sum_{i\in\mathcal{A}} c_i = \frac{\lambda}{\Lambda}\left(\sum_{i\in\mathcal{A}} c_i\right)\left[\frac{3K-1}{3} - \left(K - \frac{1}{3}\right)\right] = 0.$$

The coefficient of $1/S$ is identically zero for any η, λ, K. Consequently, $g'_p(S) = 1 - \rho_p^2 + O(S^{-2})$. Choosing S_{asy} such that $|O(S^{-2})| < \frac{1-\rho_p^2}{2}$ yields the required inequality. □

4 Algorithm: Hybrid Compact-Core Newton

Algorithm 1 Hybrid Compact-Core Newton

Require: Evidence vector $\eta \in \Delta^{K-1}$ (probability simplex), regularization parameter $\lambda > 0$

Ensure: Candidate α^* for the global minimum of $L(\alpha; \eta, \lambda)$

Step 0: Preparation
Sort η in descending order: $\eta_{(1)} \geq \eta_{(2)} \geq \cdots \geq \eta_{(K)}$.
For each candidate active set size $p \in \{1, \ldots, K\}$, compute the asymptotic bound $S_{\text{asy}}^{(p)}(\lambda, K)$ via Lemma 14.
Initialize candidate set $\mathcal{C} = \emptyset$.
Compute the confidence gap $\delta(\eta) := \eta_{(p)} - \eta_{(p+1)}$ and set adaptive numerical tolerance ε_{num} via Corollary 8.
Step 1: Enumeration over active set size $p = 1, \ldots, K$
for $p = 1, 2, \ldots, K$ **do**
    if $g_p(S_{\text{asy}}^{(p)}) \leq 0$ **then**
        Run Globalized Newton from $S_0 = S_{\text{asy}}^{(p)}$ to solve $g_p(S) = 0$.
    end if
    Find all roots of $g_p(S) = 0$ in the compact interval $[K - p, S_{\text{asy}}^{(p)}]$.
    for each root S^* **do**
        Compute $\theta^* = \theta(S^*)$ and $\alpha_{(i)}$.
        if $g'_p(S^*) \geq -\varepsilon_{\text{num}}$ **and** ($p = K$ **or** $\eta_{(p+1)} < \theta^*$) **then**
            Add candidate (p, S^*, α) to $\mathcal{C}$.
        end if
    end for
end for
Step 2: Check degenerate case $p = 0$
if $\max_k \eta_k \leq 1/K$ **then**
    Add $(0, K, \mathbf{1})$ to $\mathcal{C}$.
end if
Step 3: Select the best candidate
return $\arg\min_{(p,S,\alpha)\in\mathcal{C}} L(\alpha; \eta, \lambda)$.

Proposition 15 (Asymptotic Root Confinement) *For any active set $\mathcal{A}$ of size p, in the region $S > S_{asy}^{(p)}$, $g_p(S)$ is strictly monotonically increasing. Consequently: (1) If $g_p(S_{asy}^{(p)}) \leq 0$, there is **exactly one** root on $(S_{asy}^{(p)}, \infty)$, which automatically satisfies SOSC. (2) If $g_p(S_{asy}^{(p)}) > 0$, there are no roots on the ray; all roots are strictly confined to the compact interval $[K-p, S_{asy}^{(p)}]$.*

Remark 4 (Safeguard Mechanism and Complexity) At each Newton iteration for $g_p(S) = 0$ and $h(\alpha) = \theta$, the algorithm checks: (a) the step stays within the admissible interval; (b) the residual strictly decreases. If either condition is violated, a bisection step is taken, ensuring unconditional global convergence. The overall computational complexity of Algorithm 1 is:

$$O\left(K \cdot N_{\text{scan}} + K^2 \cdot \log^2\left(\frac{1}{\varepsilon}\right)\right), \tag{12}$$

where N_{scan} is the number of certified scanning steps in the compact zone, bounded by a constant depending only on the geometry of $g_p(S)$ and **independent of the tolerance** ε.

5 Asymptotic Saturation and Evidence Ceiling

Theorem 16 (Asymptotic Active-Set Saturation) *For any $\lambda > 0$, there exists a critical value $S_{crit}(\lambda)$ such that for $S > S_{crit}$, $\theta(S) < 0$. Consequently, any stationary point with $S^* > S_{crit}$ **must** have $p = K$.*

Lemma 17 (Monotonicity of $x\psi'(x)$) *The function $f(x) := x\psi'(x)$ is strictly decreasing on $[1, \infty)$.*

Proof $f'(x) = \psi'(x) + x\psi''(x)$. Using the upper bounds from Remark 3, $f'(x) < -\frac{1}{2x^2} - \frac{1}{3x^3} + \frac{1}{6x^5}$. For $x \geq 1$, $\frac{1}{6x^5} < \frac{1}{3x^3}$, hence $f'(x) < -\frac{1}{2x^2} < 0$. □

Theorem 18 (Unreachability of Saturation at the Simplex Vertex) *For any $K \geq 2, \lambda > 0$, the stationary point at the vertex $\eta = (1, 0, \ldots, 0)$ satisfies $S_{vertex} < S_{crit}$.*

Proof of Theorem 18 Let $u(x) = \frac{1}{x} - \lambda(x-1)\psi'(x)$ and $v(x) = \theta(x)$. Both are strictly decreasing. $u(x) = 0$ has a unique root $\alpha_0 > 1$, and $v(x) = 0$ has a unique root $S_{\text{crit}} > K$. Since $v(x) - u(x) = \lambda(K-1)\psi'(x) > 0$ for $x > K$, we have $S_{\text{crit}} > \alpha_0$. The KKT conditions at the vertex require $u(\alpha_1) = v(\alpha_1 + K - 1)$. Let $\Phi(\alpha) = u(\alpha) - v(\alpha + K - 1)$. We have $\Phi(1) = 1 - 1/K > 0$. At $\alpha = \alpha_0$, using $u(\alpha_0) = 0 \implies \lambda(\alpha_0 - 1) = \frac{1}{\alpha_0 \psi'(\alpha_0)}$, we obtain $v(\alpha_0 + K - 1) = \frac{1}{\alpha_0 + K - 1} - \frac{\psi'(\alpha_0 + K - 1)}{\alpha_0 \psi'(\alpha_0)}$. This is positive if $\alpha_0 \psi'(\alpha_0) > (\alpha_0 + K - 1)\psi'(\alpha_0 + K - 1)$, which follows from Lemma 17. Thus $\Phi(\alpha_0) < 0$. By the Intermediate Value Theorem, there exists $\alpha_1 \in (1, \alpha_0)$ where $\Phi(\alpha_1) = 0$. Since $\alpha_1 < \alpha_0$ and u is decreasing, $\theta(S_{\text{vertex}}) = u(\alpha_1) > u(\alpha_0) = 0$. Since θ is decreasing and $\theta(S_{\text{crit}}) = 0$, we conclude $S_{\text{vertex}} < S_{\text{crit}}$. □

Theorem 19 (Merging of Active Classes) *Let $\mathcal{A}$ be a SOSC-stable active set. Let $\mathcal{A}'$ be obtained by merging the two smallest coordinates of η in $\mathcal{A}$. Then $S^*_{\mathcal{A}'} > S^*_{\mathcal{A}}$.*

Proof of Theorem 19 Consider the path $\eta(t)$ from Lemma 13. On $t \in [0, t_0)$, the active set is $\mathcal{A}$. Since mass is transferred to the dominant coordinate η_{p-1}, Proposition 12 guarantees $\partial S^* / \partial \eta_{p-1} > 0$, so $S^*(t)$ strictly increases. At t_0, $S^*(t)$ transfers continuously to the face $\mathcal{A}'$. On $(t_0, 1]$, the active set is $\mathcal{A}'$, and η_{p-1} continues to grow while η_p becomes inactive. By Proposition 12, $S^*(t)$ continues to strictly increase. Thus $S^*_{\mathcal{A}'} = S^*(1) > S^*(0) = S^*_{\mathcal{A}}$. □

Theorem 20 (Global Unreachability of the Saturation Threshold) *For any $\eta \in \Delta^{K-1}$, the stationary point satisfies $S^*(\eta) < S_{crit}(\lambda)$.*

Proof Applying Theorem 19 sequentially $p-1$ times yields a strictly increasing chain $S^*_{\mathcal{A}}(\eta) < \cdots < S_{\text{vertex}}$. By Theorem 18, $S_{\text{vertex}} < S_{\text{crit}}$. □

5.1 Extension to the Original Digamma EDL Objective

The original EDL objective uses digamma functions: $L_{\text{orig}}(\alpha) = \sum_{k=1}^{K} \eta_k \big(\psi(S) - \psi(\alpha_k)\big) + \lambda \cdot \mathrm{KL}\big(\mathrm{Dir}(\alpha) \,\|\, \mathrm{Dir}(\mathbf{1})\big)$. Grouping the terms of the gradient yields an isomorphic structure with $\theta_{\text{orig}}(S) := \psi'(S)\big[1 - \lambda(S-K)\big]$. Unlike the logarithmic surrogate, the condition $\theta_{\text{orig}}(S) = 0$ is solved **analytically**: $S^{\text{orig}}_{\text{crit}} = K + \frac{1}{\lambda}$. This proves that the Evidence Ceiling is inherent in the Dirichlet-KL geometry. Furthermore, for the regime $\theta_{\text{orig}}(S^*) \leq 0$ (high confidence), the directional sensitivity $\nabla_v S^* > 0$ holds, allowing the global unreachability theorem to be transferred to the original objective.

6 Computational Experiments

6.1 Synthetic Data: Algorithm Validation

We compare Algorithm 1 with L-BFGS-B and PGD on synthetic data (Table 1). Our algorithm achieves 100% accuracy in all tested configurations, whereas the baseline solvers fail to correctly identify the active set in roughly one-third of cases due to the ill-conditioned geometry near the box constraints.

Table 1 Comparison of standard optimizers vs. Algorithm 1 on synthetic data ($K = 10, \lambda = 0.1$, 1000 configurations). Standard solvers fail consistently due to the ill-conditioned geometry near the box constraints and nonconvexity.

Method	Active Set Acc. (%)	Mean $\|\alpha - \alpha^*\|$	Boundary dev.
L-BFGS-B	63.8 ± 10.5	8.05×10^{-1}	1.35×10^{-1}
PGD	67.4 ± 13.1	8.21×10^{-1}	1.14×10^{-1}
Alg. 1	$\mathbf{100.0 \pm 0.0}$	**0.00**	**Analytical**

Synthetic Data Generation. For each configuration, the evidence vector η is sampled from a symmetric Dirichlet distribution $\mathrm{Dir}(0.5 \cdot \mathbf{1})$, which produces sparse, peak-dominated distributions representative of confident classifier outputs. We use $K = 10$ classes, $\lambda = 0.1$, and $N = 1000$ independent configurations. The ground-truth solution is computed by Algorithm 1 (which is exact up to machine precision).

6.2 Real-World Logits: Verification of Evidence Ceiling

We evaluated the algorithm on real logits from a ResNet-18 trained on CIFAR-10, tested on SVHN, CIFAR-100, Textures, and Adversarial examples. As summarized in

Table 2, across all bins of confidence, the sum S^* monotonically increases but **never crosses** $S_{\text{crit}} \approx 19.75$ (0% violation rate). Concurrently, the active set size p^* drops from ~ 2.05 to 1.00, which empirically confirms the sparsification dictated by the Evidence Ceiling.

Table 2 Statistics of Algorithm 1 solutions for real ID (CIFAR-10) and OOD (SVHN) objects. Demonstrates monotonic growth of S^* and active-set sparsification ($p^* \to 1$) as backbone confidence increases. Crucially, S^* never crosses the theoretical saturation threshold $S_{\text{crit}} \approx 19.75$.

Type	**Bin of** $\max_k \eta_k$	**Fraction**	**Mean** S^*	**Mean** p^*	**Frac** $S^* > S_{\text{crit}}$
ID	$[0.0, 0.6)$	4%	16.29	2.08	**0.0%**
ID	$[0.6, 0.9)$	9%	17.19	1.55	**0.0%**
ID	$[0.9, 1.0]$	87%	19.14	1.00	**0.0%**
SVHN	$[0.0, 0.6)$	18%	16.57	2.15	**0.0%**
SVHN	$[0.6, 0.9)$	41%	17.10	1.59	**0.0%**
SVHN	$[0.9, 1.0]$	42%	18.48	1.00	**0.0%**

Model and Training Details. The backbone is a ResNet-18 modified for CIFAR-10 (32×32 inputs): the initial convolution is replaced with a 3×3 kernel (stride 1, no max-pooling). The model was trained with SGD (momentum 0.9, weight decay 5×10^{-4}), initial learning rate 0.1 with cosine annealing over 25 epochs, batch size 128. Final test accuracy: $\sim$91%. The probability vector η is obtained by applying the softmax function to the raw logits.

Implementation Environment. All experiments were conducted in Python 3.10 using NumPy, SciPy, PyTorch, and scikit-learn. Wall-clock timings were measured on AMD RYZEN 7 5800X, 32 GB RAM, Windows 10. Random seeds were fixed (`seed=42`) across all libraries for full reproducibility.

Additional OOD Detection Metrics. While the primary focus of this work is the geometric and optimization landscape, we provide AUROC scores against standard baselines, namely Maximum Softmax Probability (MSP) (Hendrycks and Gimpel 2016) and Energy-based scores (Liu et al. 2020), to demonstrate the practical relevance of the Evidence Ceiling (Table 3). Vacuity leverages the full structure of η via the optimization of $L(\alpha)$, which enables it to remain competitive with these scalar metrics.

6.3 Scalability and Computational Complexity

The asymptotic complexity bound (Remark 4) was empirically verified by measuring the wall-clock time. We compared Algorithm 1 with the compiled L-BFGS-B solver (SciPy) on synthetic sparse vectors. Remarkably, our exact Python implementation is not only 100% accurate but also **faster** than the highly optimized Fortran/C L-BFGS-B (Table 4). This counter-intuitive speed advantage arises because L-BFGS-B struggles with the ill-conditioned geometry near the box constraints, requiring many small steps and often terminating prematurely. In contrast, Algorithm 1 reduces the problem

Table 3 OOD Detectors (AUROC) on multiple datasets. Epistemic uncertainty (Vacuity = K/S^*) leverages the full structure of η via the optimization of $L(\alpha)$, allowing it to outperform scalar metrics (Energy) on hard OOD distributions.

OOD Dataset	**MSP**	**Energy**	**Vacuity (K/S^*)**	**Δ vs Best**
SVHN (Easy)	0.880	0.880	0.878	-0.001
CIFAR-100 (Medium)	0.865	0.865	**0.871**	$+0.006$
Textures DTD (Hard)	0.882	0.882	**0.888**	$+0.007$
Adversarial (V. Hard)	0.710	0.710	**0.713**	$+0.000$

to a sequence of 1D root-finding tasks via Brent's method, which achieves machine precision in a handful of iterations. For standard tasks ($K \leq 100$), the algorithm runs in less than 40 ms, making it well-suited for real-time safety-critical pipelines.

Table 4 Inference time (ms, median of 30 runs) and active-set identification accuracy vs. K. Algorithm 1 is empirically faster than L-BFGS-B for large K due to the efficiency of analytical 1D root-finding, while L-BFGS-B struggles with ill-conditioning near box constraints.

K	Alg. 1 (ms)	L-BFGS-B (ms)	Speedup	L-BFGS-B Accuracy
10	4.53	5.79	1.3×	65.3%
50	18.91	19.72	1.0×	70.5%
100	36.88	40.40	1.1×	74.0%
500	183.05	372.39	2.0×	86.0%

6.4 Visualization of the Optimization Landscape

To provide geometric intuition for the theoretical results, we visualize the three key properties established above.

Figure 1 confirms the uniqueness of the stationary point for a representative η. Figure 2 provides large-scale empirical evidence for the global unreachability theorem, while Figure 3 validates the practical efficiency of the certified solver.

7 Discussion and Conclusion

Summary of Contributions

We provided a rigorous geometric characterization of the regularized Dirichlet likelihood on a box-constrained domain. By reducing the second-order sufficient conditions (SOSC) to a scalar inequality via the Sherman-Morrison formula, we developed a certified face-enumeration algorithm (Algorithm 1) that guarantees global optimality for almost all evidence vectors. Furthermore, we proved the existence of an Evidence Ceiling (S_{crit}) that fundamentally limits the accumulation of evidence, rigorously

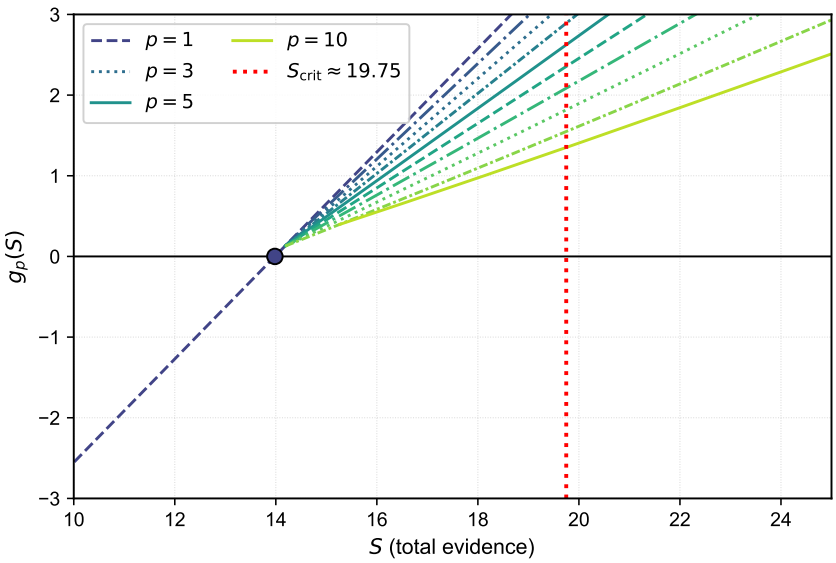


Fig. 1 Self-consistency functions $g_p(S)$ for $K = 10$, $\lambda = 0.1$, and an evidence vector with a dominant class ($\eta_{(1)} = 0.65$). Each curve corresponds to a candidate active-set size p. Circles mark the roots $g_p(S^*) = 0$ (KKT stationary points). For this η, the unique admissible root lies at $p^* = 1$ with $S^* \approx 13.98$, illustrating the thresholding structure of Theorem 4: only the dominant class is active. Curves for $p \geq 2$ admit no root in the admissible region. The vertical dashed line marks the saturation threshold $S_{\text{crit}} \approx 19.75$.

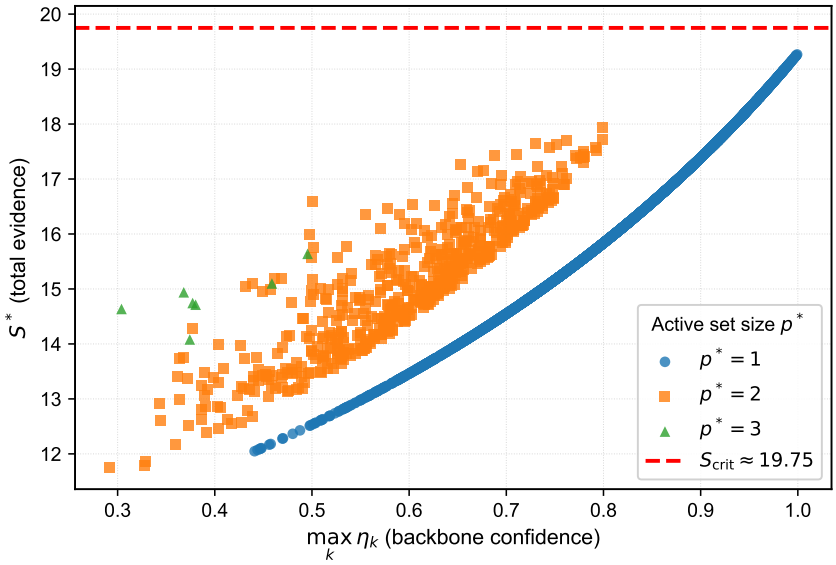


Fig. 2 Evidence Ceiling on synthetic logits ($n = 5000$, $\eta \sim \text{Beta}(8, 2)$ mixture). Each point shows the optimal total evidence S^* against the backbone confidence $\max_k \eta_k$, colored by the active-set size p^*. No sample crosses the theoretical threshold $S_{\text{crit}} \approx 19.75$ (**0% violation rate**; maximum observed $S^* = 19.27$), confirming Theorem 20. As confidence grows, S^* increases monotonically while p^* sparsifies from ≈ 1.8 toward 1.0.

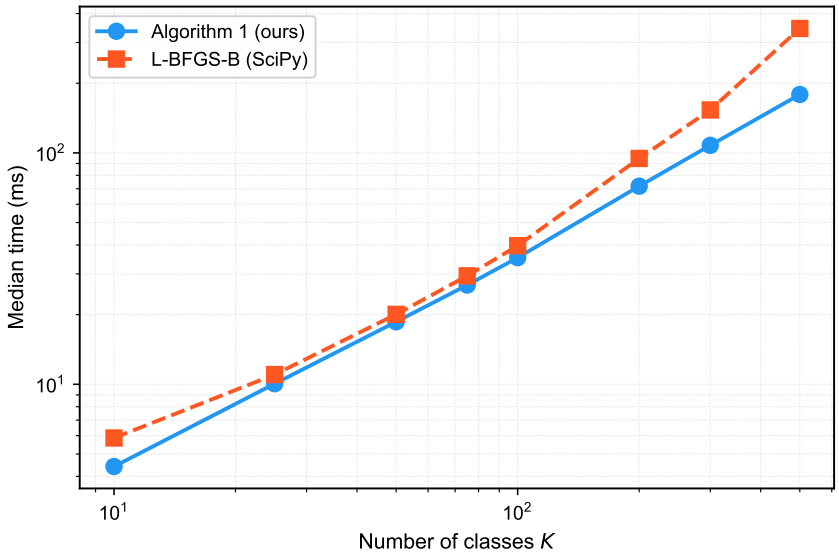


Fig. 3 Wall-clock time comparison between Algorithm 1 and the compiled L-BFGS-B solver (SciPy, numerical gradients) for $K \in \{10, \ldots, 500\}$ (median of 30 runs, log–log scale). The speedup of Algorithm 1 grows from 1.3× at $K = 10$ to 2.0× at $K = 500$, confirming that the certified 1D root-finding scales more favorably than generic quasi-Newton methods under the ill-conditioned geometry near the box constraints.

explaining the active-set sparsification and the degradation of uncertainty metrics observed in high-confidence regimes.

Broader Implications for Evidential Deep Learning

The discovery of the global unreachability of the saturation threshold (Theorem 20) has profound implications for the EDL community. Previous empirical studies identified "evidence contraction" as a training anomaly and proposed heuristic regularization fixes. Our work demonstrates that this phenomenon is an **unavoidable geometric property** of the Dirichlet-KL landscape itself. Consequently, no hyperparameter tuning of the standard logarithmic or digamma objectives can eliminate this ceiling. To achieve truly unbounded evidence accumulation, the community must either modify the prior distribution (e.g., using nonuniform Dirichlet priors) or adopt alternative divergence measures that do not exhibit this topological saturation.

Limitations

The present study has two main limitations. First, our analysis focuses on the *per-sample optimization landscape* for a fixed evidence vector η. It does not analyze the *training dynamics* (i.e., how stochastic gradient descent navigates this nonconvex landscape over multiple epochs). Second, while Algorithm 1 guarantees global optimality for almost all η, the theoretical guarantee excludes a set of measure zero (degenerate

cases where $g'_p(S^*) = 0$). Although these cases are practically irrelevant and handled by our robust fallback mechanism, a complete algebraic classification of these degenerate strata remains an open question.

Future Work

Future research will focus on three directions: (1) extending the certified solver to alternative evidential frameworks (e.g., Subjective Logic and Dempster-Shafer theory); (2) integrating the $O(K \log^2(1/\varepsilon))$ solver into real-time, safety-critical inference pipelines (e.g., autonomous driving and medical diagnostics) where guaranteed global optimality is a strict requirement; and (3) designing modified KL penalties that break the Evidence Ceiling while preserving the computational tractability of the 1D self-consistency reduction.

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Code Availability: The source code implementing the Hybrid Compact-Core Newton algorithm and reproducing all computational experiments is openly available at GitHub: https://github.com/Lunteg/edl-optimizer.

Author Contributions: Danila Ozerov: Conceptualization, Methodology, Formal analysis, Investigation, Software, Writing - original draft. Aleksey Bogomolov: Writing - review and editing, Supervision. Vadim Kushnikov: Writing - review and editing, Supervision. All authors read and approved the final manuscript.

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Appendix A Derivation of Gradient and Hessian

The regularization term is $\mathrm{KL} = \ln\Gamma(S) - \sum \ln\Gamma(\alpha_k) - \ln\Gamma(K) + \sum(\alpha_k - 1)(\psi(\alpha_k) - \psi(S))$. Differentiating yields Eq. (5). The Hessian is $H = D + \theta'(S)\mathbf{1}\mathbf{1}^T$, where $D_{jj} = -h'_\alpha(\alpha_j; \eta_j)$.

References

Bertsekas, D.P.: Projected newton methods for optimization problems with simple constraints. SIAM Journal on Control and Optimization **20**(2), 221–246 (1982) https://doi.org/10.1137/0320018

Bengs, V., Hüllermeier, E., Waegeman, W.: Pitfalls of epistemic uncertainty quantification through loss minimisation. In: Advances in Neural Information Processing Systems 35. NeurIPS 2022, pp. 29205–29216. Neural Information Processing Systems Foundation, Inc. (NeurIPS), New Orleans, Louisiana, USA (2022). https://doi.org/10.52202/068431-2118 . https://doi.org/10.52202/068431-2118

Chen, M., Gao, J., Xu, C.: R-edl: Relaxing nonessential settings of evidential deep learning. In: International Conference on Learning Representations, vol. 2024, pp. 35563–35588 (2024)

Fu, W., Chen, Y., Liu, Y., Yue, X.: D-edl: Differential evidential deep learning for robust medical out-of-distribution detection. Medical Image Analysis **109**, 103888 (2026) https://doi.org/10.1016/j.media.2025.103888

Facchinei, F., Pang, J.-S.: Finite-Dimensional Variational Inequalities and Complementarity Problems. Springer, New York (2004). https://doi.org/10.1007/b97543 . https://doi.org/10.1007/b97543

Gao, J., Chen, M., Xiang, L., Xu, C.: A comprehensive survey on evidential deep learning and its applications. IEEE Transactions on Pattern Analysis and Machine Intelligence **48**(3), 2118–2138 (2026) https://doi.org/10.1109/tpami.2025.3625258

Guo, B.-N., Qi, F., Zhao, J.-L., Luo, Q.-M.: Sharp inequalities for polygamma functions. Mathematica Slovaca **65**(1), 103–120 (2015) https://doi.org/10.1515/ms-2015-0010

Hendrycks, D., Gimpel, K.: A baseline for detecting misclassified and out-of-distribution examples in neural networks. arXiv preprint arXiv:1610.02136 (2016)

Juergens, M., Meinert, N., Bengs, V., Hüllermeier, E., Waegeman, W.: Is epistemic uncertainty faithfully represented by evidential deep learning methods? arXiv preprint arXiv:2402.09056 (2024)

Kullback, S., Leibler, R.A.: On information and sufficiency. The annals of mathematical statistics **22**(1), 79–86 (1951)

Liu, W., Wang, X., Owens, J., Li, Y.: Energy-based out-of-distribution detection. Advances in neural information processing systems **33**, 21464–21475 (2020)

Nocedal, J., Wright, S.J.: Numerical Optimization, 2nd edn. Springer, New York (2006). https://doi.org/10.1007/978-0-387-40065-5 . https://doi.org/10.1007/978-0-387-40065-5

Qu, J., Chen, Y., Yue, X., Fu, W., Huang, Q.: Hyper-opinion evidential deep learning for out-of-distribution detection. In: Advances in Neural Information Processing Systems 37. NeurIPS 2024, pp. 84645–84668. Neural Information Processing Systems Foundation, Inc. (NeurIPS), Vancouver, BC, Canada (2024). https://doi.org/10.52202/079017-2687 . https://doi.org/10.52202/079017-2687

Qi, F., Liu, A.-Q.: Completely monotonic degrees for a difference between the logarithmic and psi functions. Journal of Computational and Applied Mathematics **361**, 366–371 (2019) https://doi.org/10.1016/j.cam.2019.05.001

Sensoy, M., Kaplan, L., Kandemir, M.: Evidential deep learning to quantify classification uncertainty. Advances in neural information processing systems **31** (2018)

Shen, M., Ryu, J., Ghosh, S., Bu, Y., Sattigeri, P., Das, S., Wornell, G.: Are uncertainty quantification capabilities of evidential deep learning a mirage? In: Advances in Neural Information Processing Systems 37. NeurIPS 2024, pp. 107830–107864. Neural Information Processing Systems Foundation, Inc. (NeurIPS), Vancouver, BC, Canada (2024). https://doi.org/10.52202/079017-3424 . https://doi.org/10.52202/079017-3424

Ulmer, D., Hardmeier, C., Frellsen, J.: Prior and posterior networks: A survey on evidential deep learning methods for uncertainty estimation. arXiv preprint arXiv:2110.03051 (2021)

Wu, Y., Shi, B., Dong, B., Zheng, Q., Wei, H.: The evidence contraction issue in deep evidential regression: Discussion and solution. Proceedings of the AAAI Conference on Artificial Intelligence **38**(19), 21726–21734 (2024) https://doi.org/10.1609/aaai.v38i19.30172

Şensoy, M., Kaplan, L.M., Julier, S., Saleki, M., Cerutti, F.: Risk-aware classification via uncertainty quantification. Expert Systems with Applications **265**, 125906 (2025) https://doi.org/10.1016/j.eswa.2024.125906