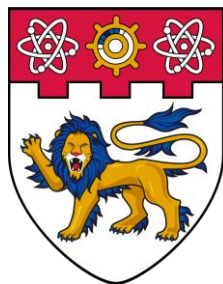


Convolutional Fenchel–Young Loss

Convex Smooth Losses with Linear Surrogate Regret



Yuzhou Cao ¹



Han Bao ²



Lei Feng ³



Bo An ^{1,4}



Learning vs. Evaluation

Evaluation stage: Performance measuring with **discrete** loss function ℓ *w.r.t.* **discrete (finite)** prediction space $\hat{\mathcal{Y}}$ ($|\hat{\mathcal{Y}}| < +\infty$)

$$\min_{h: \mathcal{X} \rightarrow \hat{\mathcal{Y}}} R_{\ell}(h) = \mathbb{E}_{X,Y}[\ell(h(X), Y)]$$

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Learning stage: Minimization of (expected) **continuous** loss function ϕ *w.r.t.* **continuous** prediction space \mathbb{R}^d .

$$\min_{f: \mathcal{X} \rightarrow \mathbb{R}^d} R_{\phi}(f) = \mathbb{E}_{X,Y}[\phi(f(X), Y)]$$

Continuous Surrogate

Learning vs. Evaluation

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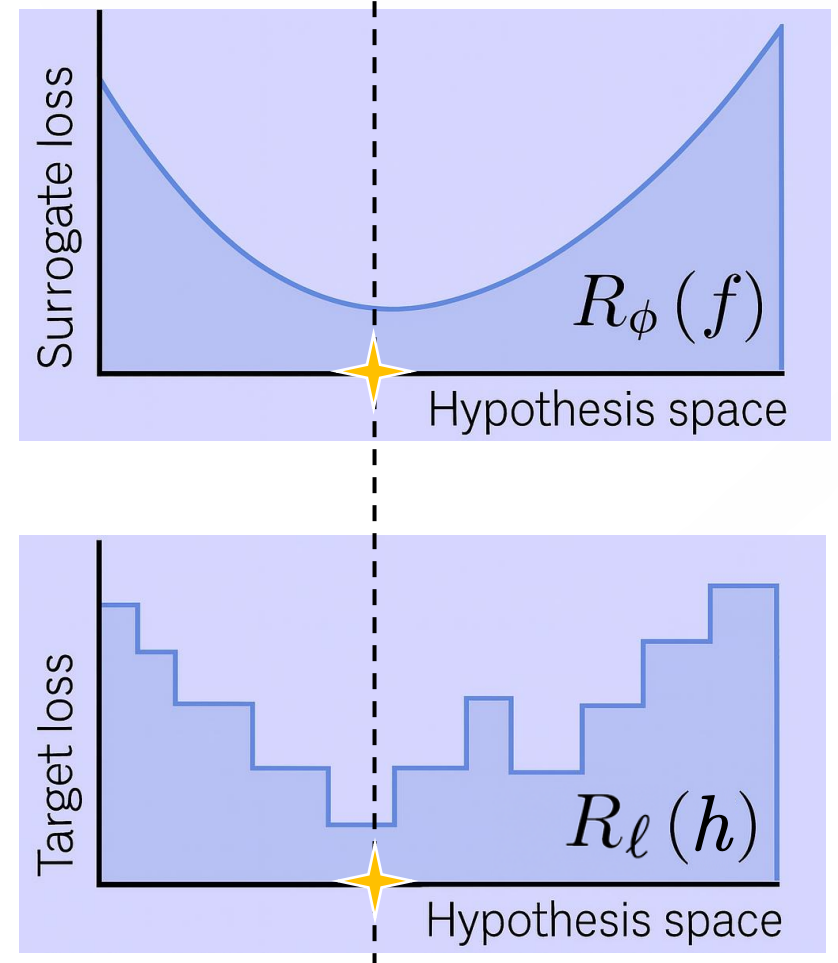
$\varphi: \mathbb{R}^d \rightarrow \hat{\mathcal{Y}}$: prediction link.

$h_{\varphi} := \varphi \circ f$: final predictive model.

What We Ask in Surrogate Loss

- Q1: Are surrogate and target losses minimized simultaneously? **Calibration/Fisher Consistency**

$$\underbrace{R_\phi(f) - \min_f R_\phi(f)}_{\text{(Surrogate) Regret}_\phi(f)} \rightarrow 0 \Rightarrow \underbrace{R_\ell(\varphi \circ f) - \min_h R_\ell(h)}_{\text{(Target) Regret}_\ell(\varphi \circ f)} \rightarrow 0$$



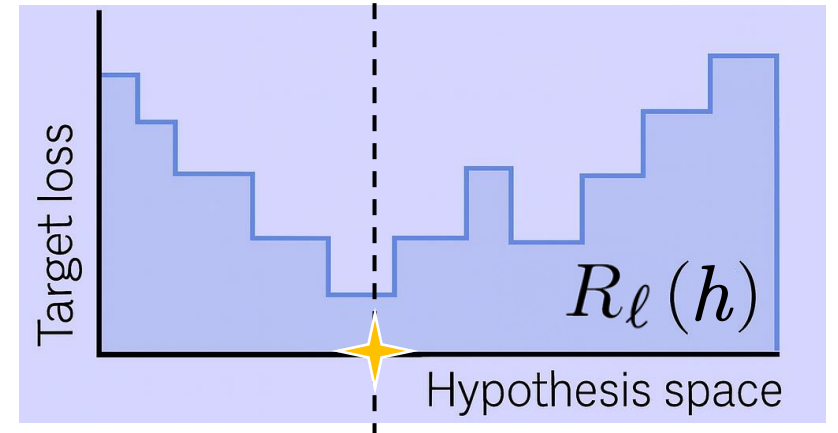
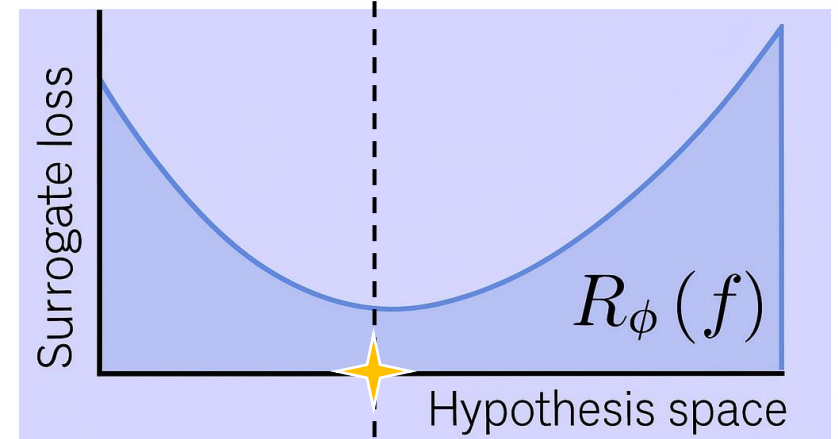
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- Q2: How the convergence of $\text{Regret}_\phi(f)$ transfers to $\text{Regret}_\ell(\varphi \circ f)$? **Surrogate Regret Bound**

$$\text{Regret}_\ell(\varphi \circ f) \leq \psi(\text{Regret}_\phi(f))$$



What We Ask in Surrogate Loss

- Q2: How the convergence of $\text{Regret}_\phi(f)$ transfers to $\text{Regret}_\ell(\varphi \circ f)$?

$$\text{Regret}_\ell(\varphi \circ f) \leq \psi(\text{Regret}_\phi(f))$$

- Two typical bounds:

- Square root:



Deteriorates target regret convergence rate!

$$\psi(*) = C \cdot \sqrt{*} \rightarrow \text{Regret}_\ell(\varphi \circ f) = \mathcal{O}_p(1/n^{p/2})$$

- Linear:



Maintains fast target regret convergence rate!

$$\psi(*) = C \cdot * \rightarrow \text{Regret}_\ell(\varphi \circ f) = \mathcal{O}_p(1/n^p)$$

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Linear ψ is desirable!

- Q3: Good Optimization Properties? **Convexity, Smoothness...**
-

A Negative Result

[FW21, Theorem 2] For surrogate-target loss pair (ϕ, ℓ) that is calibrated with surrogate regret bound ψ , if ϕ is **locally strongly convex and locally smooth**, the surrogate regret bound is **at least square-root**, e.g., there exists $\epsilon_0, C > 0$ that:

$$\psi(\epsilon) \geq C\sqrt{\epsilon}, \forall \epsilon \leq \epsilon_0$$

Includes most existing convex smooth losses:

Cross-entropy/Focal/MSE/Binary Cross-Entropy/Dice/Jaccard Index.....

A popular conjecture: convexity, smoothness, and linear surrogate regret bound are **incompatible**.

A Negative Result

A popular conjecture: convexity, smoothness, and linear surrogate regret bound are **incompatible**.

This conjecture is overturned by **Convolutional Fenchel-Young Loss!**

- Works for **any** discrete target loss.
 - Achieves a **linear surrogate regret bound**.
 - **Smooth and convex**.
 - Produces consistent **probability estimators**.
-

Target Loss Decomposition

- **Recap:** Target loss $\ell: \underset{\text{(Prediction space)}}{\hat{\mathcal{Y}}} \times \underset{\text{(Label space)}}{\mathcal{Y}} \rightarrow \mathbb{R}_{\geq 0}, |\hat{\mathcal{Y}}| = N, |\mathcal{Y}| = K.$
- **New concept:**

$$\boldsymbol{\rho} - \boldsymbol{\ell}^\rho \text{ Decomposition: } \ell(t, y) = \langle \boldsymbol{\rho}(y), \boldsymbol{\ell}^\rho(t) \rangle + c(y)$$

- Label encoding: $\boldsymbol{\rho}(y): \mathcal{Y} \rightarrow \mathbb{R}^d$
- Loss encoding: $\boldsymbol{\ell}^\rho(t): \hat{\mathcal{Y}} \rightarrow \mathbb{R}^d$
- Scalar offset: $c(y): \mathcal{Y} \rightarrow \mathbb{R}$

An (always holds) example:

$$\boldsymbol{\rho}(y) = \mathbf{e}_y \in \mathbb{R}^K, \boldsymbol{\ell}^\rho(t) = [\ell(t, 1), \dots, \ell(t, K)]^\top, c = 0.$$

Fenchel-Young Loss

- **Recap:** label encoding $\rho(y): \mathcal{Y} \rightarrow \mathbb{R}^d$

Let $\Omega: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ be a **negentropy** (convex function) with $\text{conv}\{\rho(y)\}_{y=1}^K \subseteq \text{dom}(\Omega)$
A **Fenchel-Young loss** [BMN20] $\phi_\Omega: \text{dom}(\Omega^*) \times \mathcal{Y} \rightarrow \mathbb{R}_{\geq 0}$ generated by Ω is defined as:

$$\phi_\Omega(\theta, y) = \Omega(\rho(y)) + \Omega^*(\theta) - \langle \theta, \rho(y) \rangle$$

$\Omega^*(\theta) = \sup_{\rho \in \mathbb{R}^d} \langle \theta, \rho \rangle - \Omega(\rho)$ is Fenchel conjugate.

- Quantifies discrepancy between label $\rho(y)$ and score θ via **Fenchel-Young Inequality**.

$$\Omega(\rho(y)) + \Omega^*(\theta) \geq \langle \theta, \rho(y) \rangle$$

- Always **convex**, and **smooth** with strongly convex negentropy.

Linear Surrogate Regret Bound?

- Duality between strong convexity and smoothness[KST09]:

ϕ_Ω is strongly convex if Ω is smooth.

[FW21, Theorem 2] For surrogate-target loss pair (ϕ, ℓ) that is calibrated with surrogate regret bound ψ , if ϕ is **locally strongly convex and locally smooth**, the surrogate regret bound is **at least square-root**, e.g., there exists ϵ_0 , $C > 0$ that:

$$\psi(\epsilon) \geq C\sqrt{\epsilon}, \quad \forall \epsilon \leq \epsilon_0$$

Smooth negentropy should be avoided!

Convolutional Entropy

Ordinary Negentropy $\Omega(\boldsymbol{p})$: commonly **strongly convex** & **smooth** (Square/Shannon)

Convolutional Entropy

Ordinary Negentropy $\Omega(\mathbf{p})$: commonly strongly convex & smooth (Square/Shannon)

New Concept-Task Entropy: $T(\mathbf{p}) := - \min_{t \in \hat{\mathcal{Y}}} \langle \mathbf{p}, \boldsymbol{\ell}^{\rho}(t) \rangle$

- **Recap:**

- $\ell(t, y) = \langle \boldsymbol{\rho}(y), \boldsymbol{\ell}^{\rho}(t) \rangle + c(y)$
- $T(\mathbf{p})$: a shifted negative minimum pointwise target risk.

Non-smooth but **not** strongly convex!

Convolutional Entropy

Ordinary Negentropy $\Omega(\mathbf{p})$: commonly strongly convex & smooth (Square/Shannon)

Task Entropy: $T(\mathbf{p}) := -\min_{t \in \hat{\mathcal{Y}}} \langle \mathbf{p}, \ell^\rho(t) \rangle$

Convolutional Entropy: $\Omega_T(\mathbf{p}) := (\Omega + T)(\mathbf{p})$ **strongly convex and non-smooth!**

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Why “Convolutional”?

$$\Omega_T^*(\boldsymbol{\theta}) = (\Omega^* \square T^*)(\boldsymbol{\theta}) = \inf_u \{ \Omega^*(\boldsymbol{\theta} - \mathbf{u}) + T^*(\mathbf{u}) \}$$

Infimal Convolution!

Convolutional Entropy

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$$\Omega_T^*(\boldsymbol{\theta}) = (\Omega^* \square T^*)(\boldsymbol{\theta}) = \inf_{\mathbf{u}} \{ \Omega^*(\boldsymbol{\theta} - \mathbf{u}) + T^*(\mathbf{u}) \} = \inf_{\boldsymbol{\pi} \in \Delta^N} \Omega^*(\boldsymbol{\theta} + \mathcal{L}^\rho \boldsymbol{\pi})$$
$$\mathcal{L}^\rho := [\ell^\rho(1), \dots, \ell^\rho(N)]^\top$$

Convolutional Entropy

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Conjugated Convolutional Entropy: $\Omega_T^*(\boldsymbol{\theta}) = \inf_{\boldsymbol{\pi} \in \Delta^N} \Omega^*(\boldsymbol{\theta} + \mathcal{L}^\rho \boldsymbol{\pi})$

Convolutional Fenchel-Young Loss

For strongly convex $\Omega: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ with $\text{conv}\{\boldsymbol{\rho}(y)\}_{y=1}^K \subseteq \text{dom}(\Omega)$ and $\text{dom}(\Omega^*) = \mathbb{R}^d$, a **Convolutional Fenchel-Young loss** $\phi_{\Omega_T}: \text{dom}(\Omega_T^*) \times \mathcal{Y} \rightarrow \mathbb{R}_{\geq 0}$ generated by Ω_T is:

$$\phi_{\Omega_T}(\boldsymbol{\theta}, y) = \Omega_T(\boldsymbol{\rho}(y)) + \inf_{\boldsymbol{\pi} \in \Delta^N} \Omega^*(\boldsymbol{\theta} + \mathcal{L}^\rho \boldsymbol{\pi}) - \langle \boldsymbol{\theta}, \boldsymbol{\rho}(y) \rangle$$

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- (Full domain) $\text{dom}(\phi_{\Omega_T}) = \mathbb{R}^d$.
- (Smoothness and convexity) ϕ_{Ω_T} is convex and smooth.
- (Envelope theorem)

$$\nabla_{\boldsymbol{\theta}} \min_{\boldsymbol{\pi} \in \Delta^N} \Omega^*(\boldsymbol{\theta} + \mathcal{L}^\rho \boldsymbol{\pi}) = \nabla \Omega^*(\boldsymbol{\theta} + \mathcal{L}^\rho \boldsymbol{\pi}^*), \quad \forall \boldsymbol{\pi}^* \in \Pi(\boldsymbol{\theta}) := \underset{\boldsymbol{\pi} \in \Delta^N}{\text{argmin}} \Omega^*(\boldsymbol{\theta} + \mathcal{L}^\rho \boldsymbol{\pi}^*)$$

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- **Probability estimator:** For any $\boldsymbol{\eta} \in \text{relint}(\Delta^K)$, the pointwise surrogate risk $R_{\phi_{\Omega_T}}(\boldsymbol{\theta}, \boldsymbol{\eta}) := \mathbb{E}_{Y \sim \boldsymbol{\eta}}[\phi_{\Omega_T}(\boldsymbol{\theta}, Y)]$ is minimized at $\boldsymbol{\theta}^*$:

$$\mathbb{E}_{Y \sim \boldsymbol{\eta}}[\boldsymbol{\rho}(Y)] = \nabla \Omega^*(\boldsymbol{\theta}^* + \mathcal{L}^\rho \boldsymbol{\pi}^*), \quad \forall \boldsymbol{\pi}^* \in \Pi(\boldsymbol{\theta}^*)$$

(e.g., $\mathbb{E}_{Y \sim \boldsymbol{\eta}}[\boldsymbol{\rho}(Y)] = \boldsymbol{\eta}$ when $\boldsymbol{\rho}(y) = \mathbf{e}_y \in \mathbb{R}^K$)

Surrogate Regret Analysis

- **Recap:** Surrogate regret: $\text{Regret}_{\phi_{\Omega_T}}(h) := R_{\phi_{\Omega_T}}(h) - \min_h R_{\phi_{\Omega_T}}(h)$
$$= \mathbb{E}_X \left[\underbrace{R_{\phi_{\Omega_T}}(h(X), \boldsymbol{\eta}(X)) - \min_{\boldsymbol{\theta} \in \mathbb{R}^d} R_{\phi_{\Omega_T}}(\boldsymbol{\theta}, \boldsymbol{\eta}(X))}_{\text{Regret}(h(X), \boldsymbol{\eta}(X)): \text{Pointwise Surrogate Regret}} \right]$$

- **Pointwise surrogate regret of Conv-FY loss:**

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Surrogate regret decomposition:

$$\text{Regret}_{\phi_{\Omega_T}}(\boldsymbol{\theta}, \boldsymbol{\eta}) = R_{\phi_{\Omega}}(\boldsymbol{\theta} + \mathcal{L}^{\rho} \boldsymbol{\pi}^*, \boldsymbol{\eta}) + \sum_{t=1}^N \pi_t^* \text{Regret}_{\ell}(t, \boldsymbol{\eta}), \quad \forall \boldsymbol{\pi}^* \in \Pi(\boldsymbol{\theta})$$

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Risk of FY loss $\phi_{\Omega} (\geq 0)$ Convex combination of target regret

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$$\text{Regret}_{\phi_{\Omega_T}}(\boldsymbol{\theta}, \boldsymbol{\eta}) \geq \text{Regret}_{\ell}(\hat{t}, \boldsymbol{\eta})/N$$

Linear Regret Link Construction

$$\text{Regret}_{\phi_{\Omega_T}}(\boldsymbol{\theta}, \boldsymbol{\eta}) \geq \sum_{t=1}^N \pi^*(t) \text{Regret}_{\ell}(t, \boldsymbol{\eta})$$



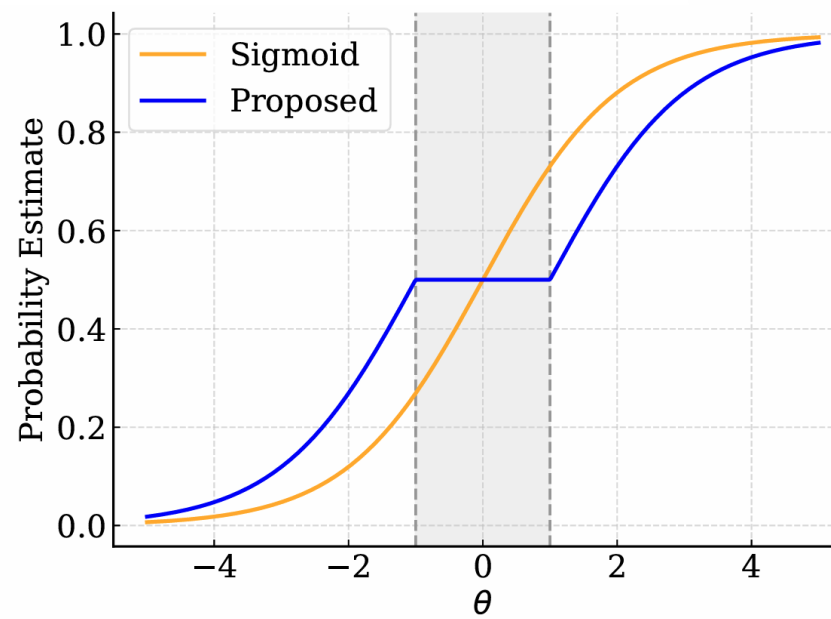
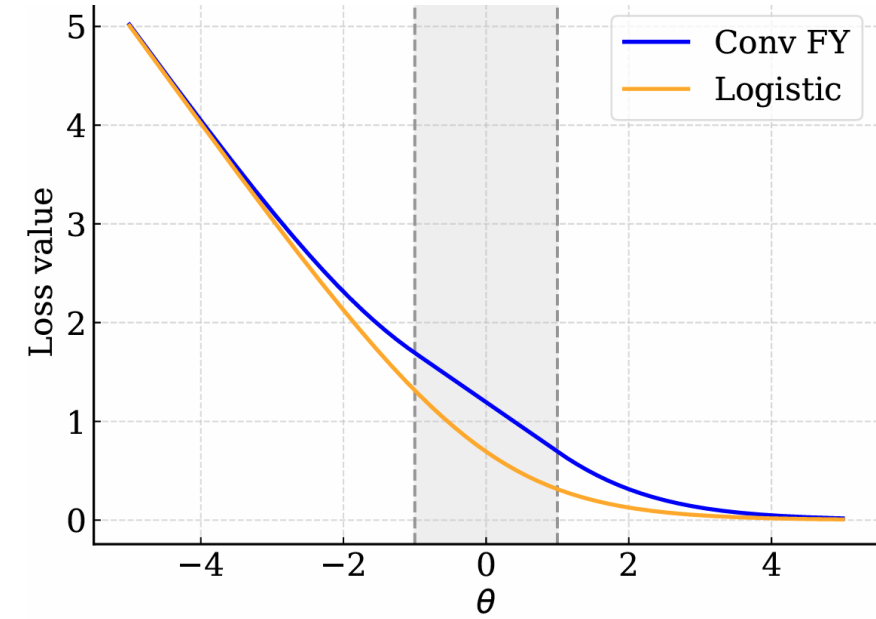
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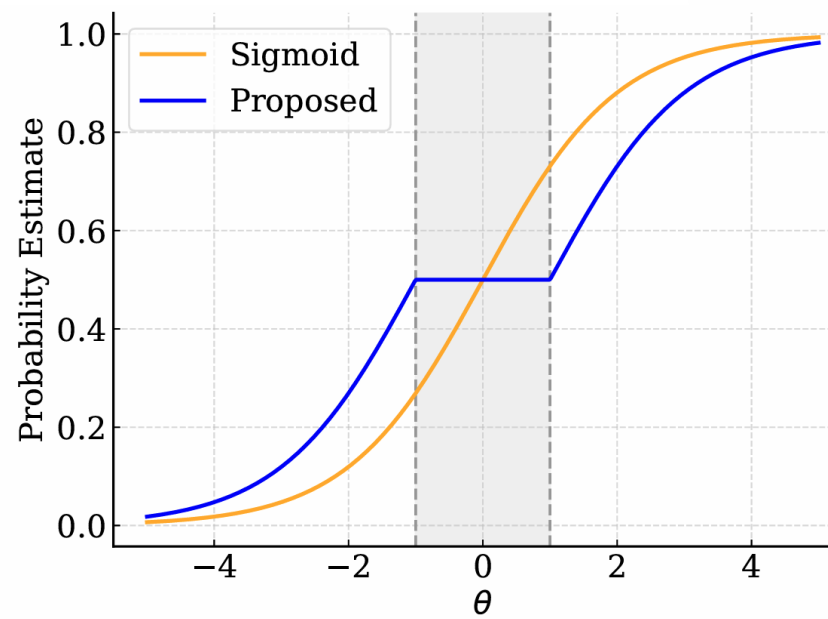
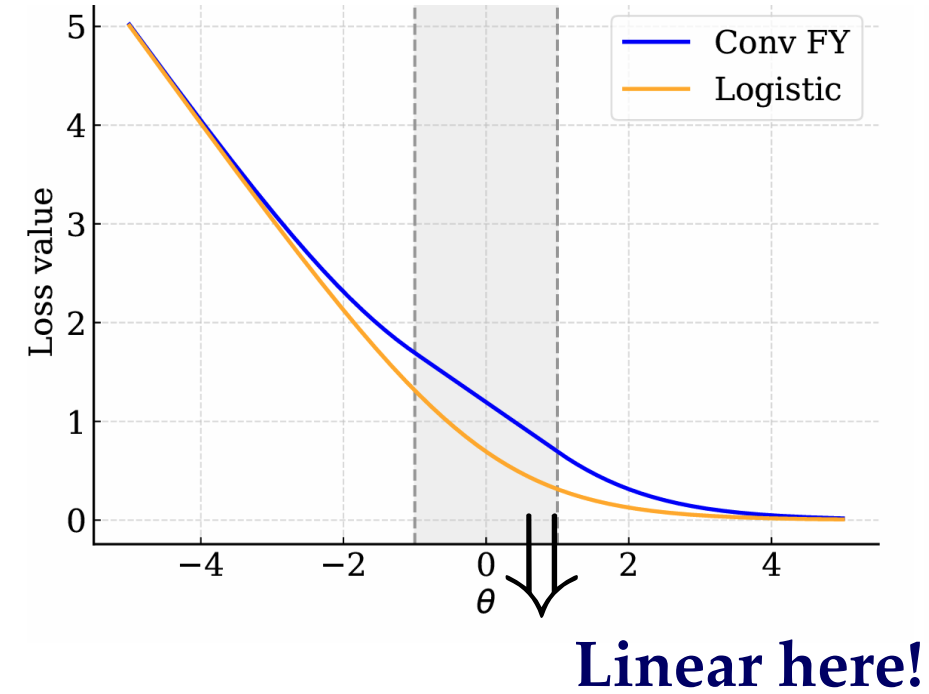
($\boldsymbol{\pi}$ -argmax link): For function $\boldsymbol{\pi}^*: \mathbb{R}^d \rightarrow \Delta^N$, if $\boldsymbol{\pi}^*(\boldsymbol{\theta}) \in \Pi(\boldsymbol{\theta})$ for any $\boldsymbol{\theta} \in \mathbb{R}^d$:

$$\text{Regret}_{\ell}(\varphi(\boldsymbol{\theta}), \boldsymbol{\eta}) \leq N \text{Regret}_{\phi_{\Omega_T}}(\boldsymbol{\theta}, \boldsymbol{\eta}), \quad \forall (\boldsymbol{\theta}, \boldsymbol{\eta}) \in \mathbb{R}^d \times \Delta^K, \quad \varphi := \operatorname{argmax} \circ \boldsymbol{\pi}^*$$

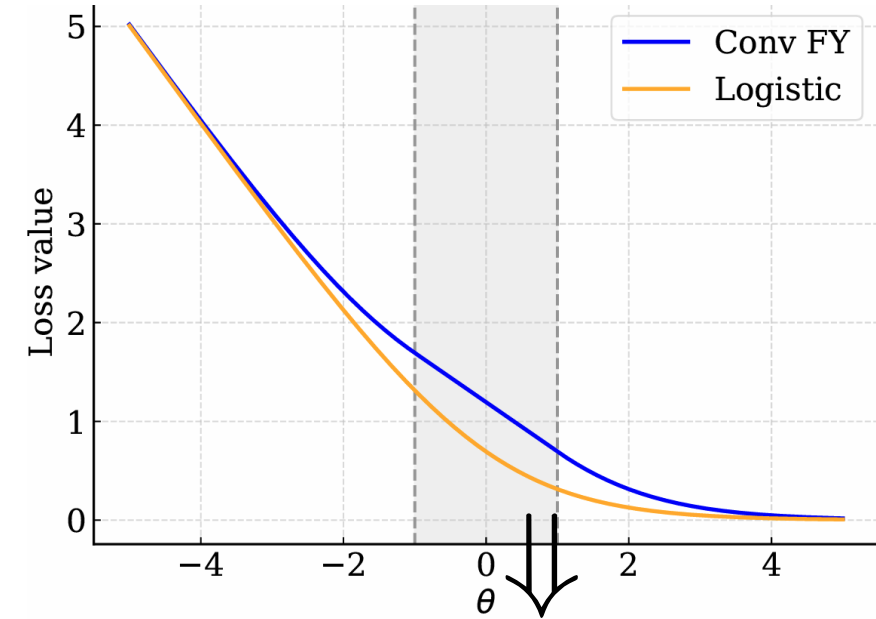
Binary Case Visualization



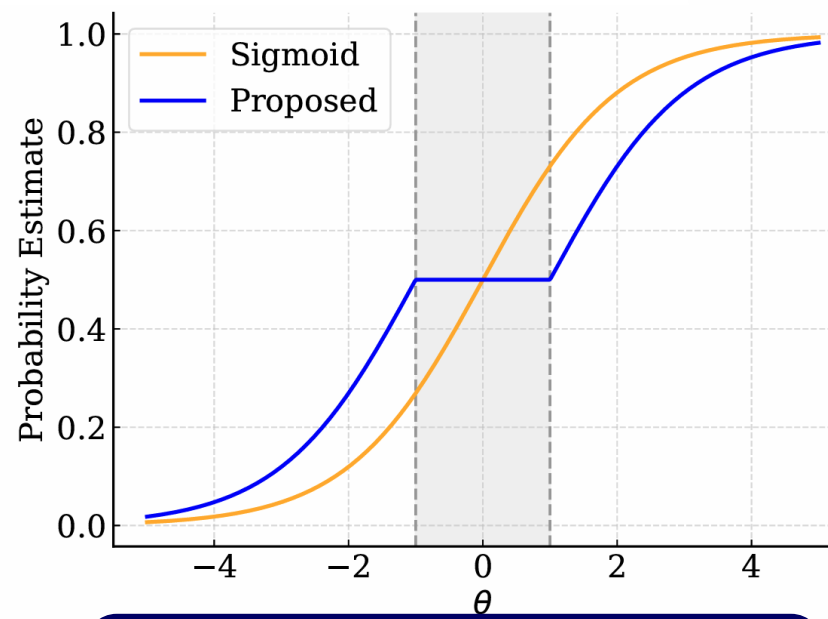
Binary Case Visualization



Binary Case Visualization



Linear here!



Circumventing sqrt bound by
injecting linearity!

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