

Proper Losses, Moduli of Convexity, and Surrogate Regret Bounds

(presented at COLT2023)

Han Bao

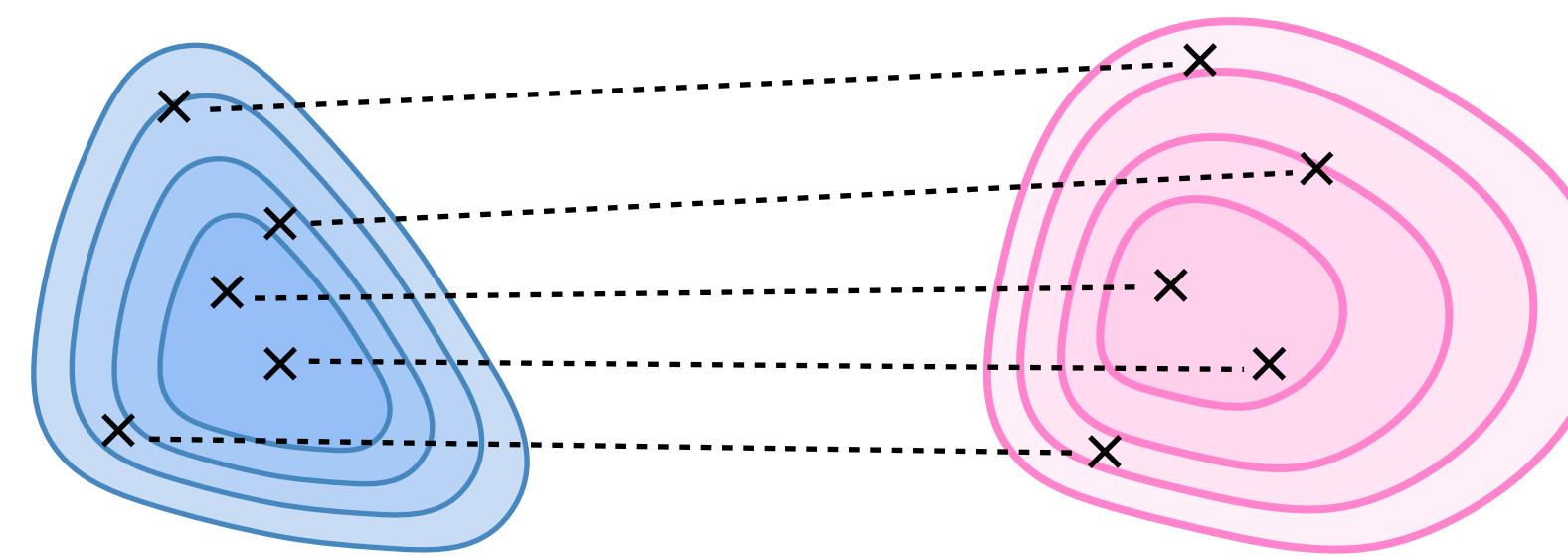
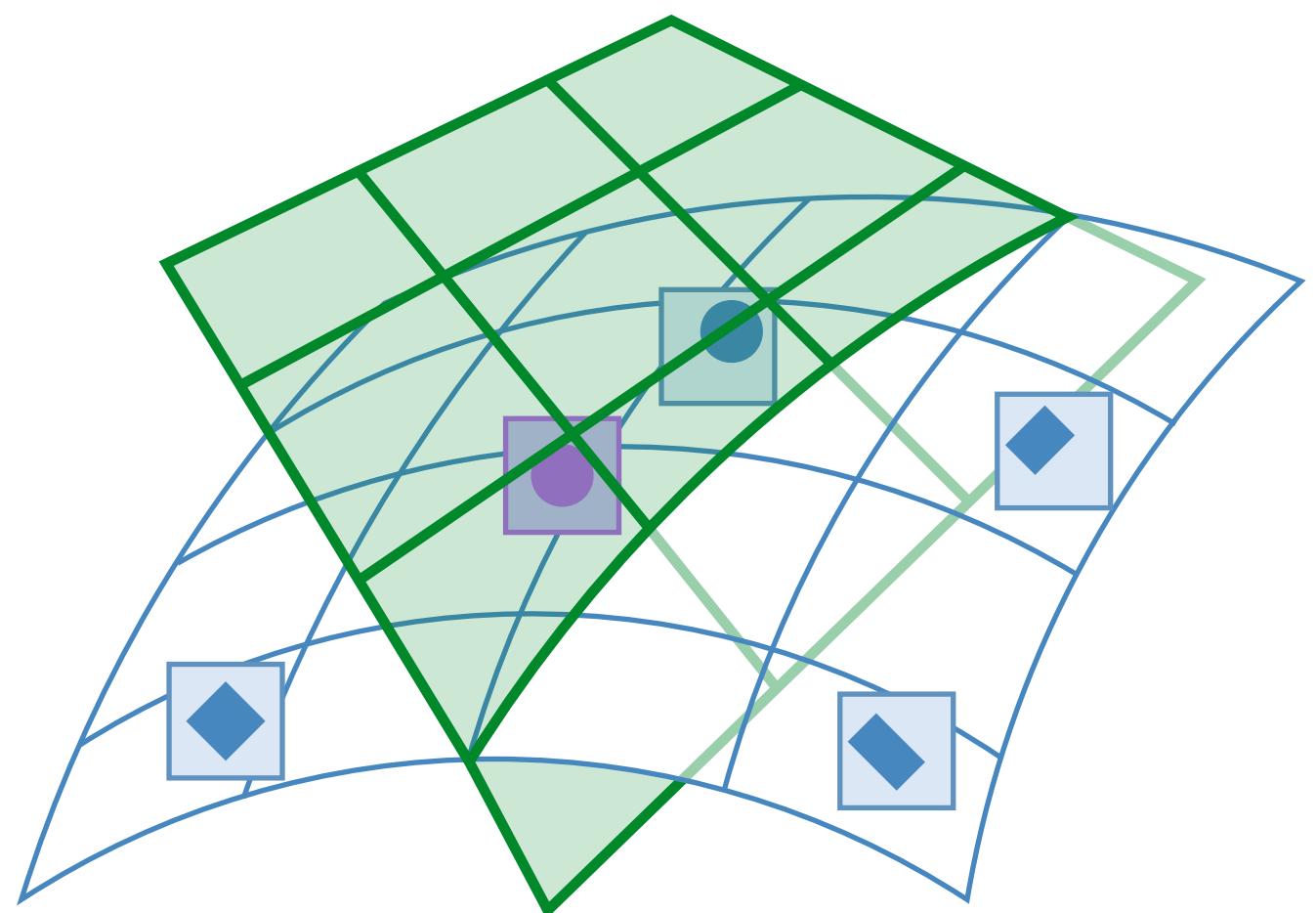
October 13rd, 2023 @ Bristol



KYOTO UNIVERSITY

Short bio | Han Bao

- 2017 April - 2022 March: Graduate student @ The University of Tokyo
- 2022 April - Current: Assistant professor @ Kyoto University (Hakubi center)
- Research keywords:
Loss function (**today's topic**), robustness, contrastive learning, optimal transport ⋯





Bandit 🇨🇦



Lervig 🇳🇴



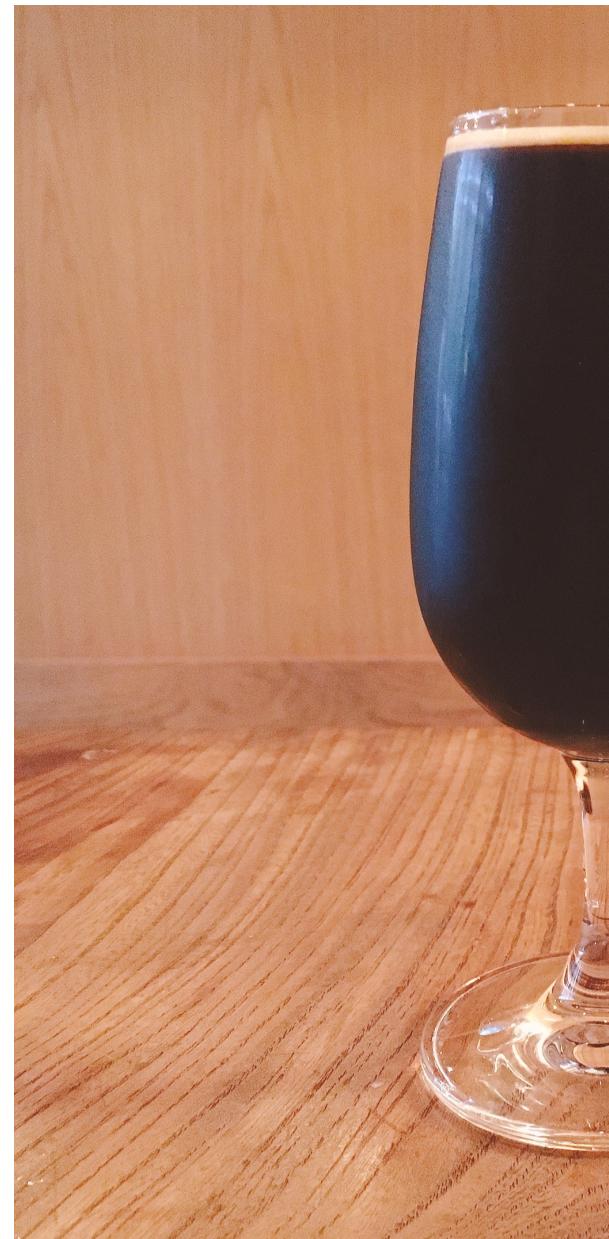
Uchu 🇯🇵



Omnipollo 🇸🇪



Bandit 🇨🇦

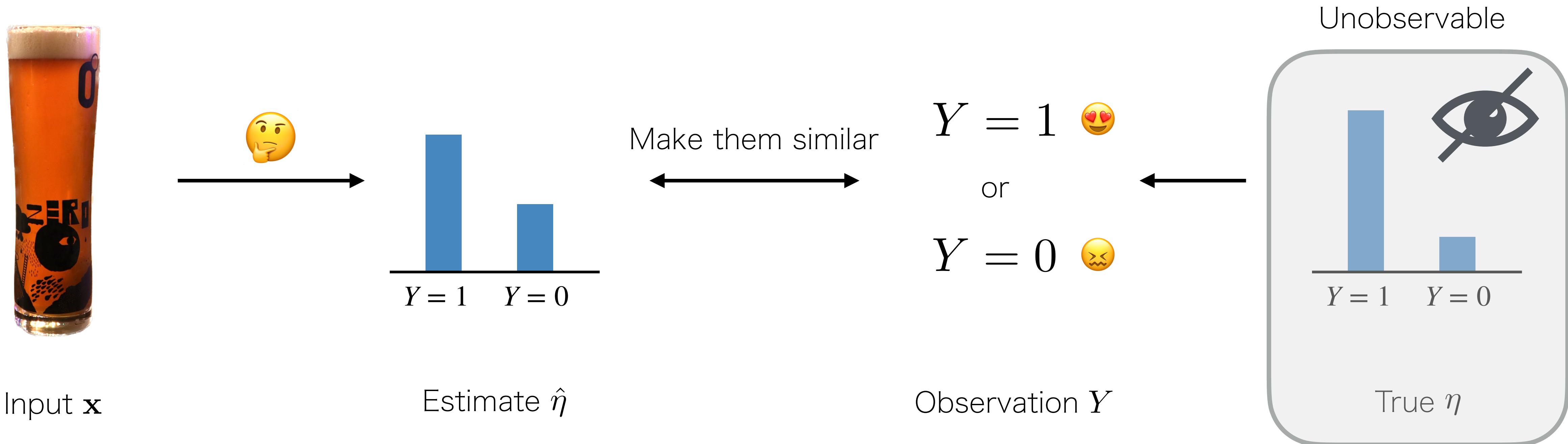


Lervi



Probabilistic prediction

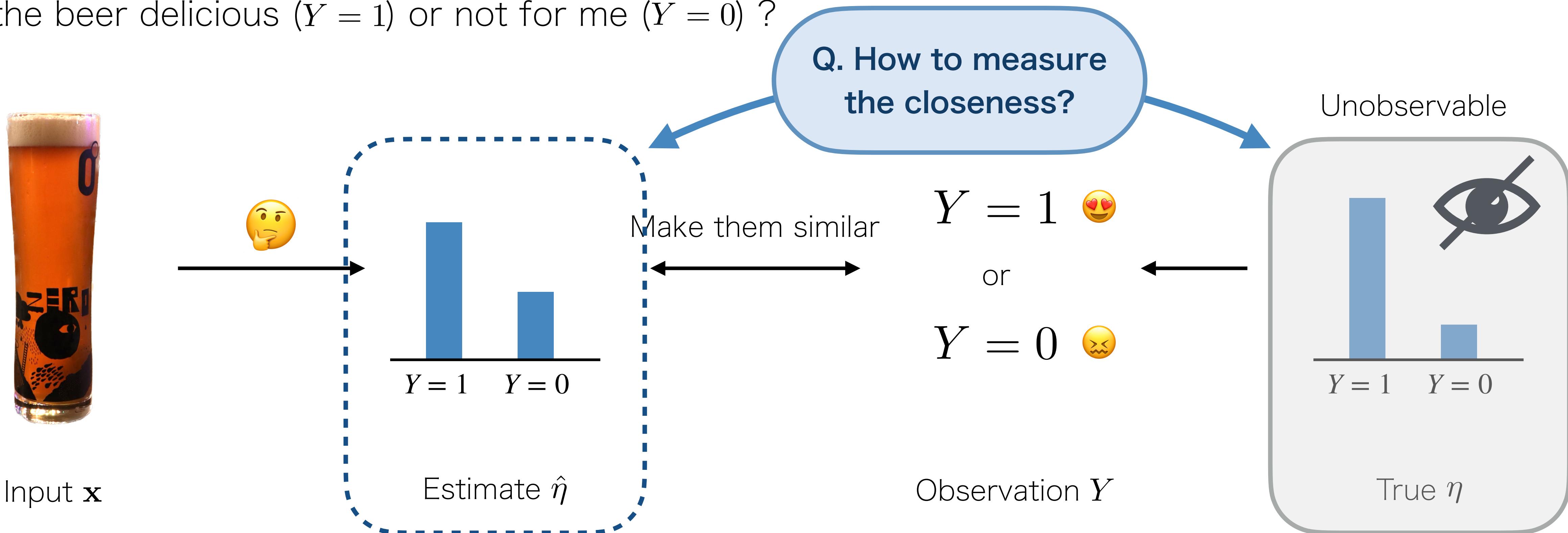
- Is the beer delicious ($Y = 1$) or not for me ($Y = 0$) ?



- We make a decision $\hat{\eta}$ that is as close to true $\eta = \mathbb{P}(Y = 1 | \mathbf{x})$ as possible

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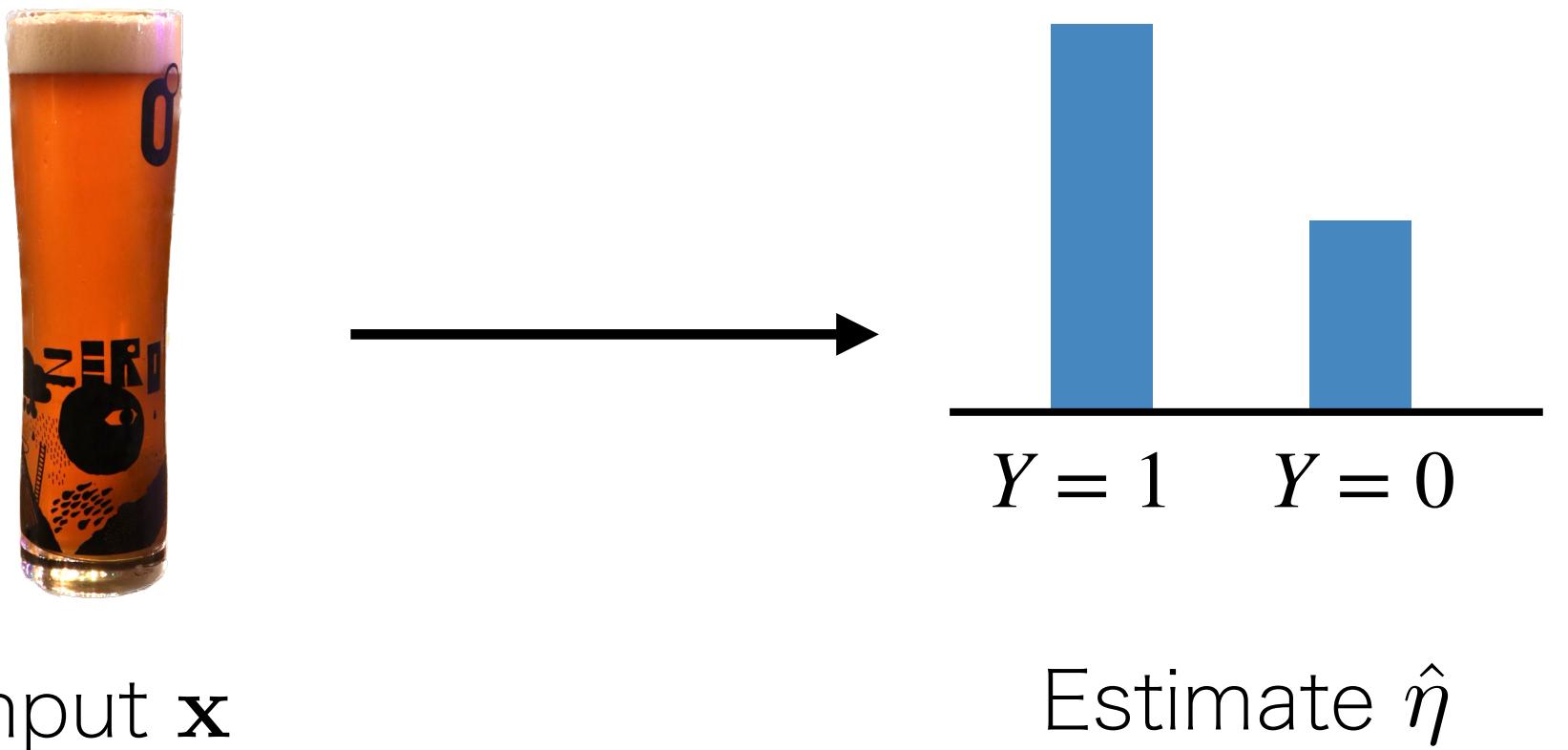
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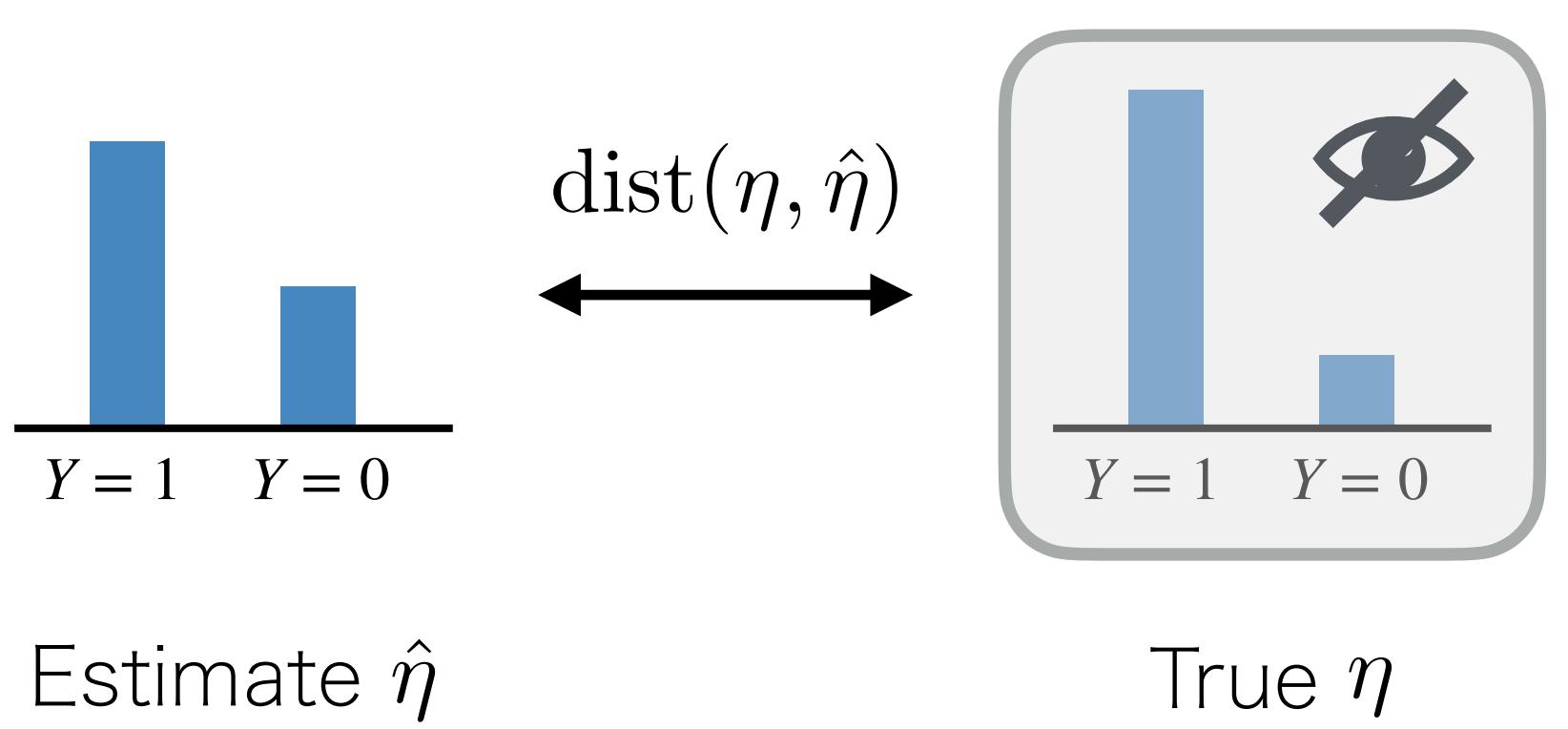
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Formulation | Probabilistic prediction

- Input: sample $\{(\mathbf{x}_i, y_i)\}_{i \in [n]}$ with binary outcome $y_i \in \{1, 0\}$
- Goal: to estimate $\eta(\mathbf{x}) = \mathbb{P}(Y = 1 \mid \mathbf{x})$
 - ❖ Output: $\hat{\eta} : \mathcal{X} \rightarrow [0, 1]$ such that $\hat{\eta} \approx \eta$

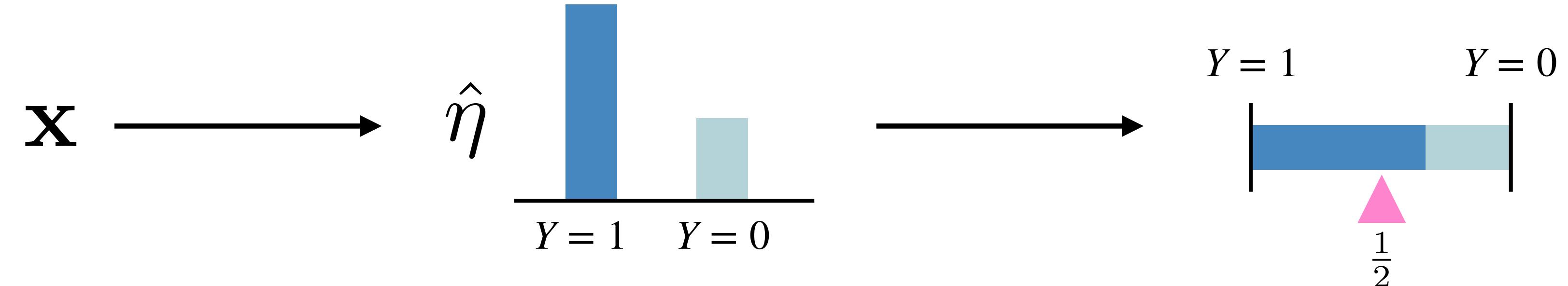


- Challenge: no observation of $\eta(\mathbf{x}_i)$
 - ❖ It is important to compute $\text{dist}(\eta(\mathbf{x}), \hat{\eta}(\mathbf{x}))$ with only $\hat{\eta}$ and y
 - ❖ Disclaimer: we do not discuss functional approximation



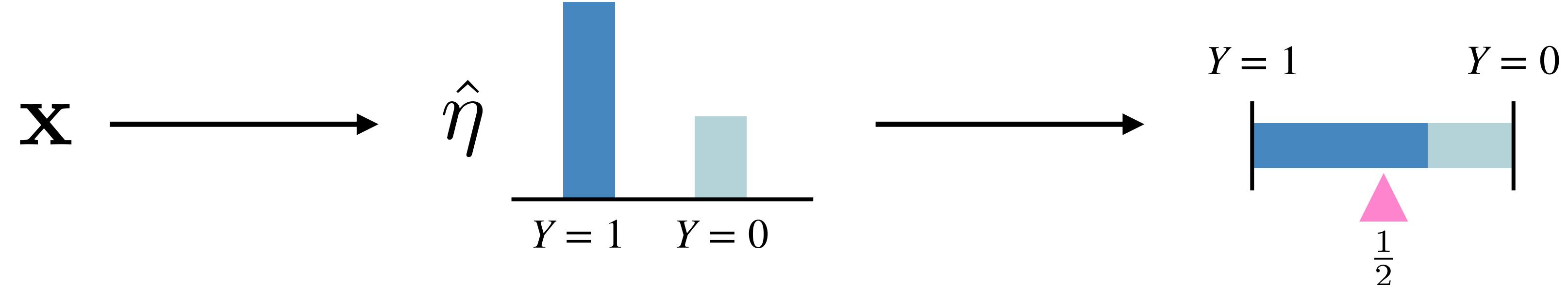
Probabilistic predictions everywhere

- Having estimated $\eta(\mathbf{x}) = \mathbb{P}(Y = 1 \mid \mathbf{x})$, many downstream tasks can be solved
- Case 1 (classification): $f^*(\mathbf{x}) = \text{sign}(\eta(\mathbf{x}) - \frac{1}{2})$



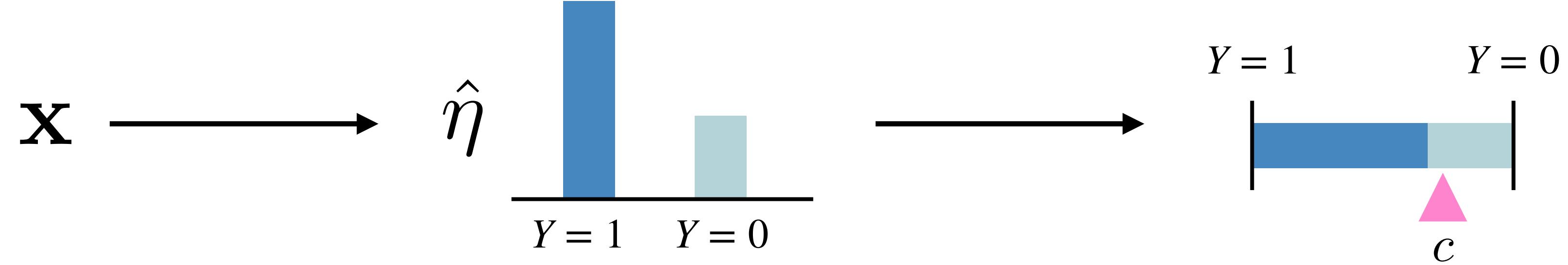
Probabilistic predictions everywhere

- Having estimated $\hat{\eta}(\mathbf{x}) = \mathbb{P}(Y = 1 \mid \mathbf{x})$, many downstream tasks can be solved
- Case 1 (classification): $f^*(\mathbf{x}) = \text{sign}(\hat{\eta}(\mathbf{x}) - \frac{1}{2})$



- Case 2 (cost-sensitive classification): $f^*(\mathbf{x}) = \text{sign}(\hat{\eta}(\mathbf{x}) - c)$ [Elkan 2001]

❖ Cost for false positives = c



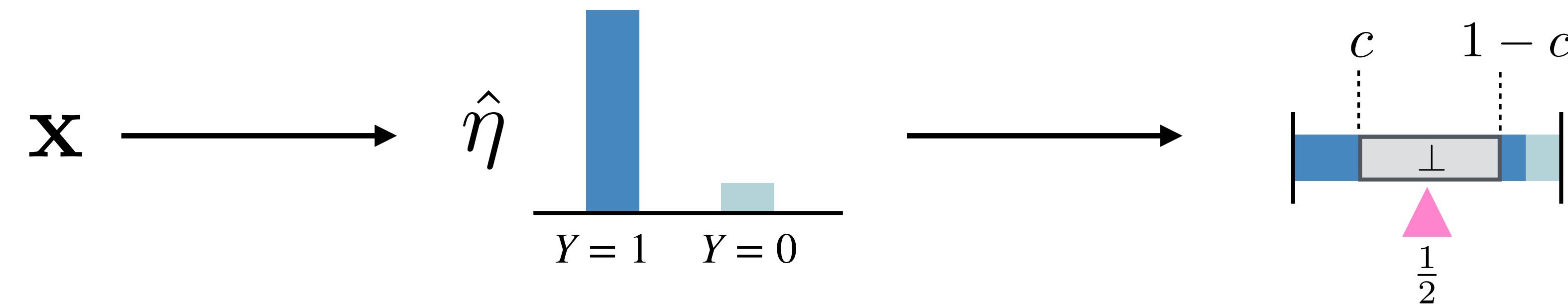
Probabilistic predictions everywhere

- Having estimated $\eta(\mathbf{x}) = \mathbb{P}(Y = 1 \mid \mathbf{x})$, many downstream tasks can be solved
- Case 3 (bipartite ranking): Higher score for positive examples than negative examples
 - ❖ $f^*(\mathbf{x}) = \iota(\eta(\mathbf{x}))$ (ι : some monotonic transform)

Probabilistic predictions everywhere

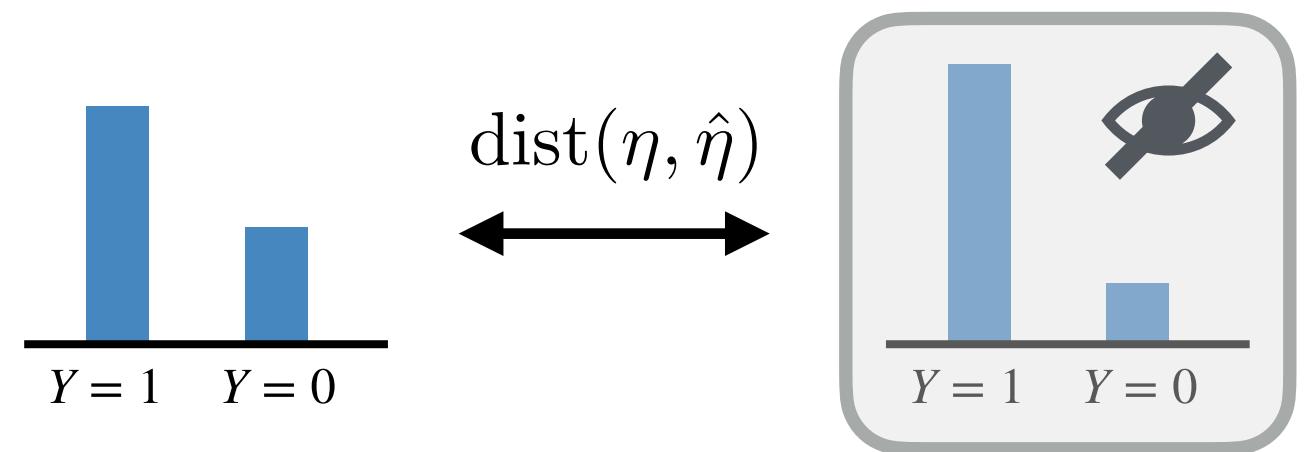
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- Case 3 (bipartite ranking): Higher score for positive examples than negative examples
 - $f^*(\mathbf{x}) = \iota(\eta(\mathbf{x}))$ (ι : some monotonic transform)
- Case 4 (learning with rejection): Agent is allowed to defer decisions to human with cost c
 - $f^*(\mathbf{x}) = \begin{cases} \perp & \text{if } c \leq \eta(\mathbf{x}) \leq 1 - c \\ \text{sign}(\eta(\mathbf{x}) - \frac{1}{2}) & \text{otherwise} \end{cases}$

[Chow 1970]



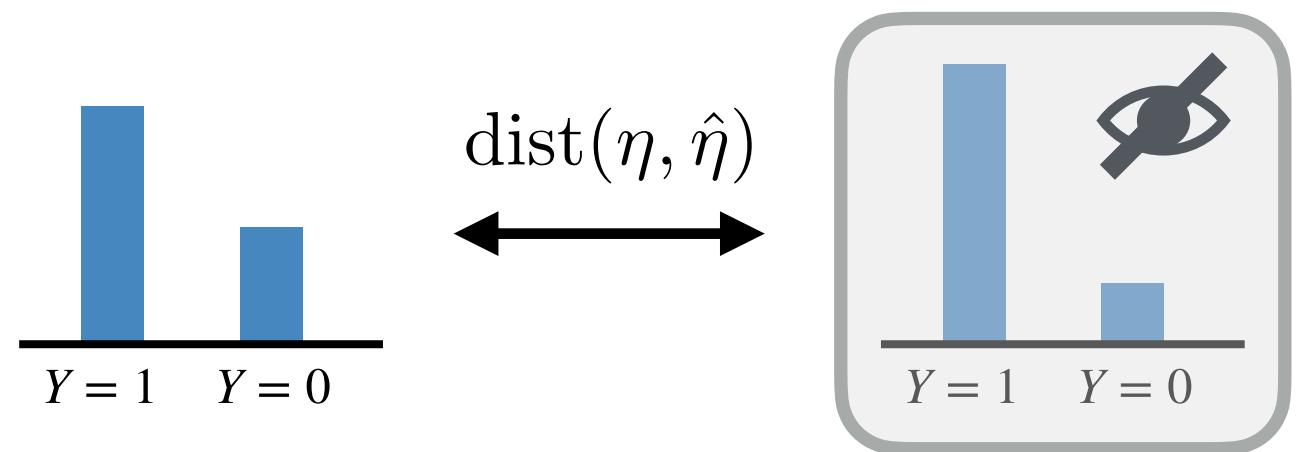
Questions

- How to compute $\text{dist}(\eta(\mathbf{x}), \hat{\eta}(\mathbf{x}))$ with only $\hat{\eta}$ and y ?



Questions

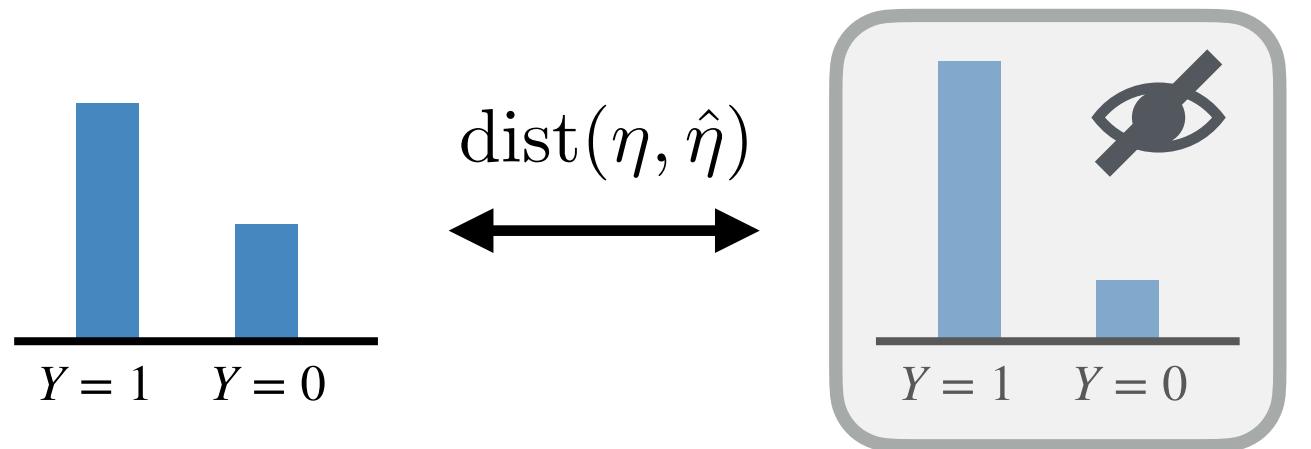
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Proper Losses

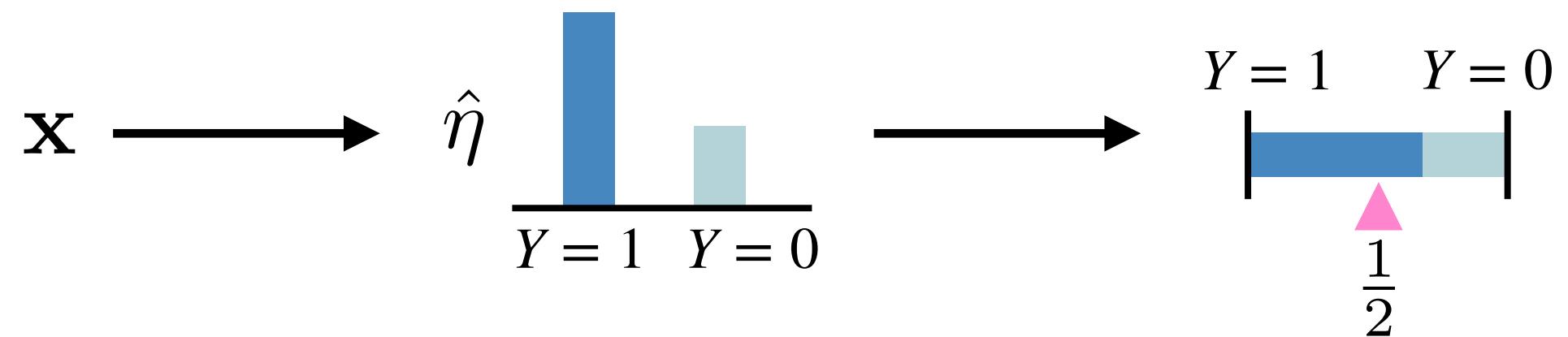
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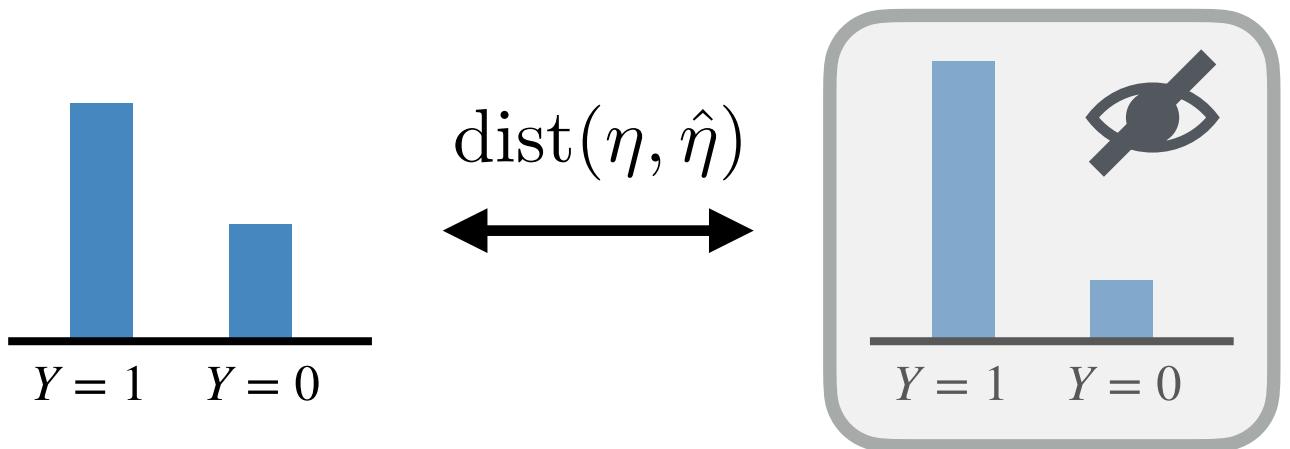
Proper Losses

- How useful is probability estimate $\hat{\eta}$ for a downstream task?



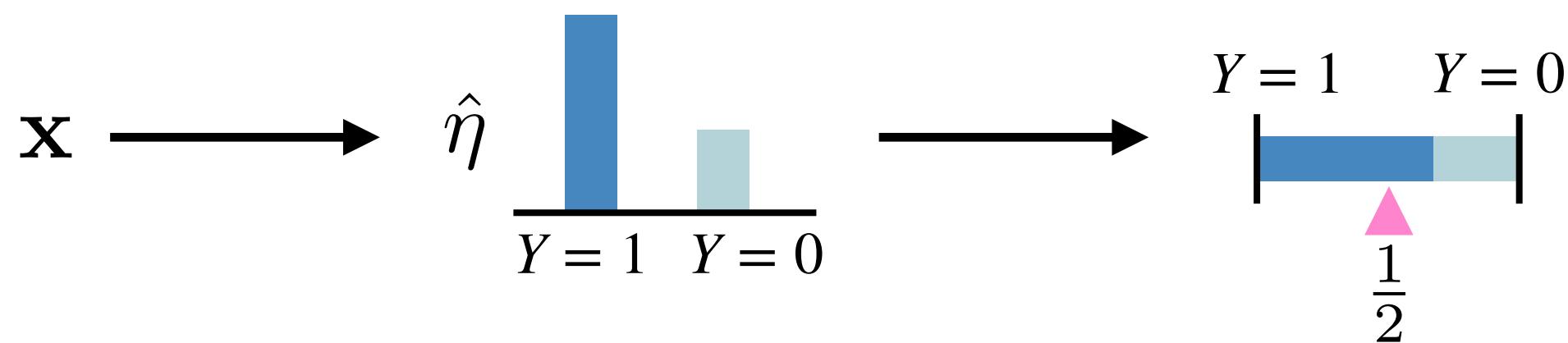
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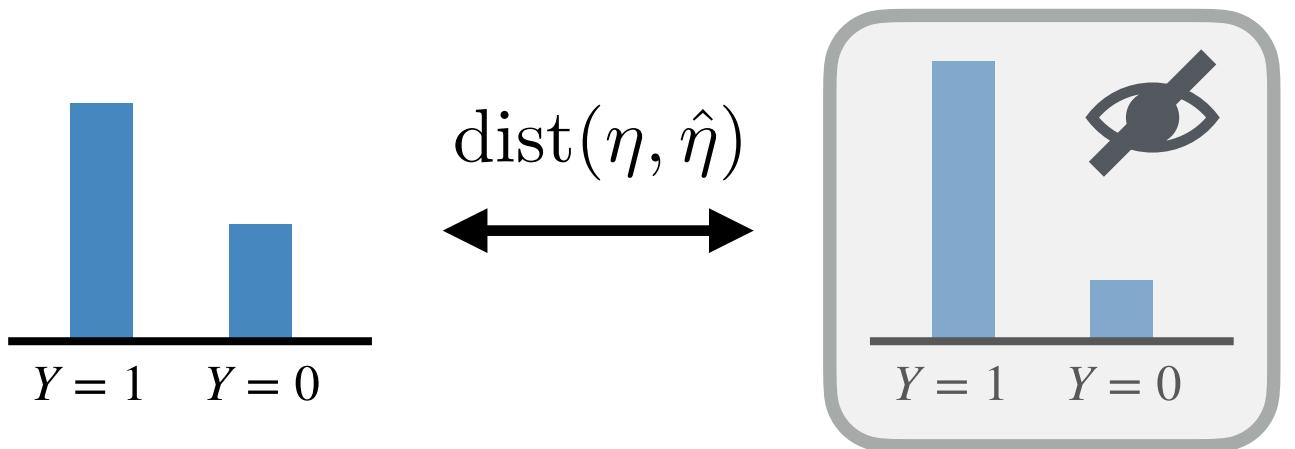
Proper Losses Surrogate Regret Bounds

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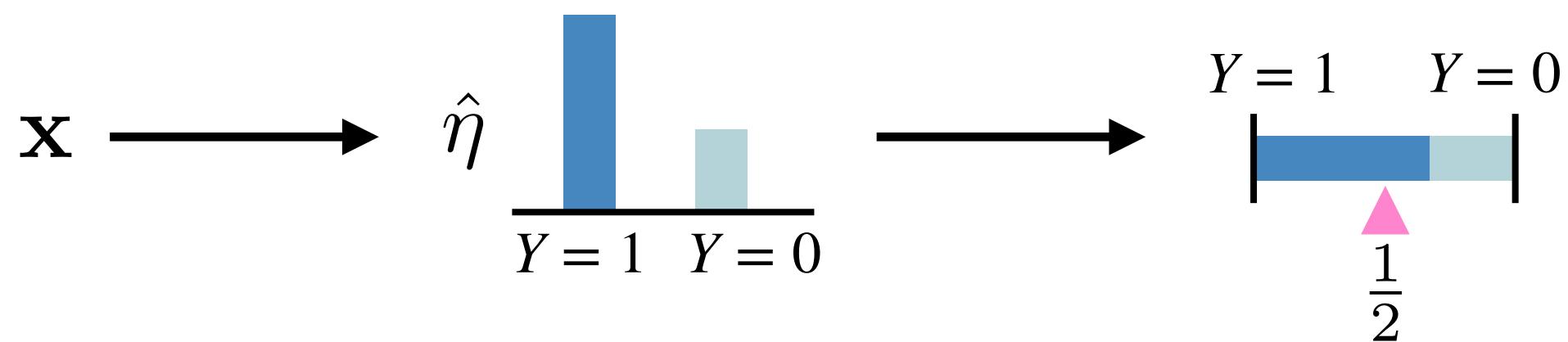
- How to compute $\text{dist}(\eta(\mathbf{x}), \hat{\eta}(\mathbf{x}))$ with only $\hat{\eta}$ and y ?



- How to derive surrogate regret bounds?

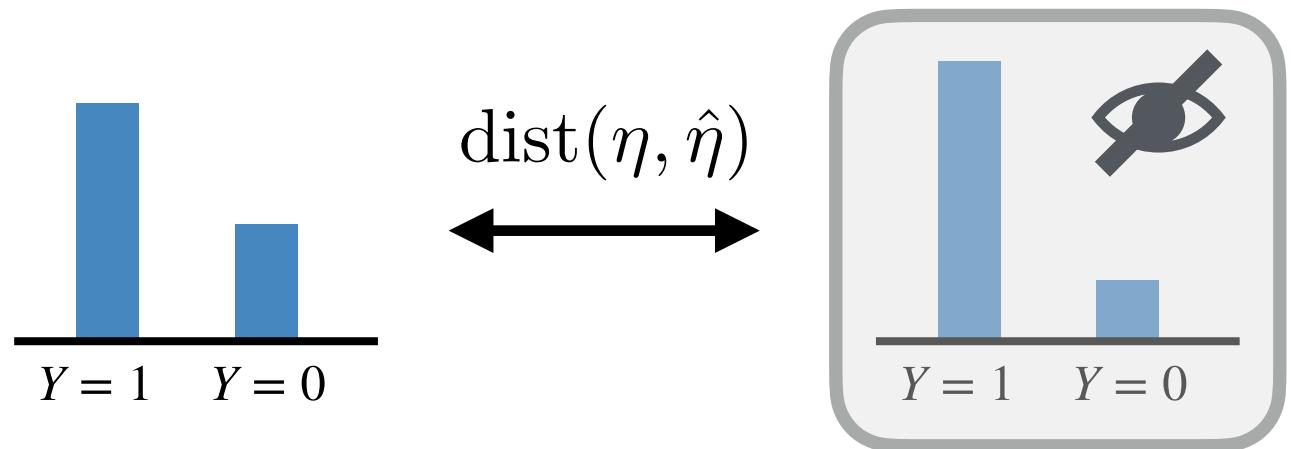
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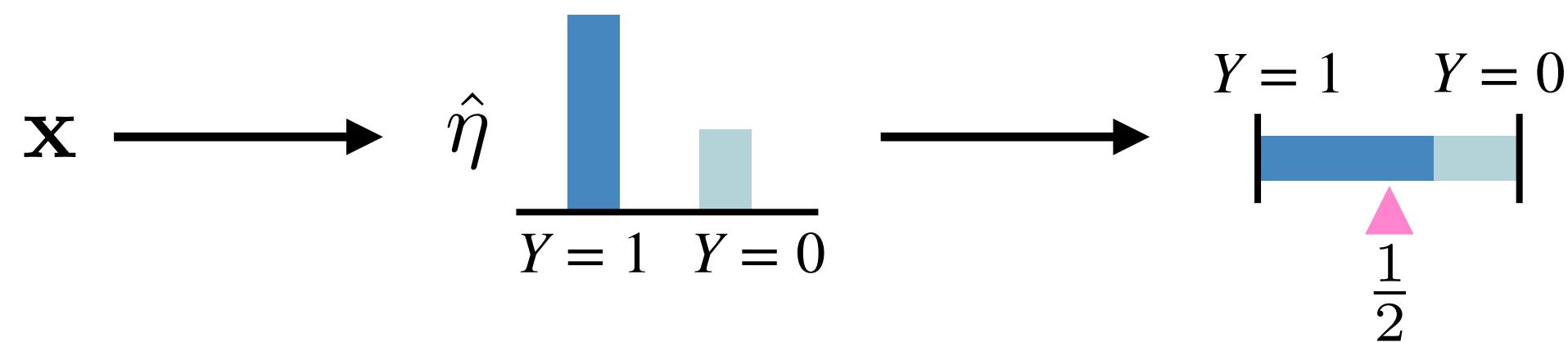
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Proper Losses, Moduli of Convexity, and Surrogate Regret Bounds

- How useful is probability estimate $\hat{\eta}$ for a downstream task?



Outline

● **Q.** How should we assess probability estimates?

- ❖ Proper losses

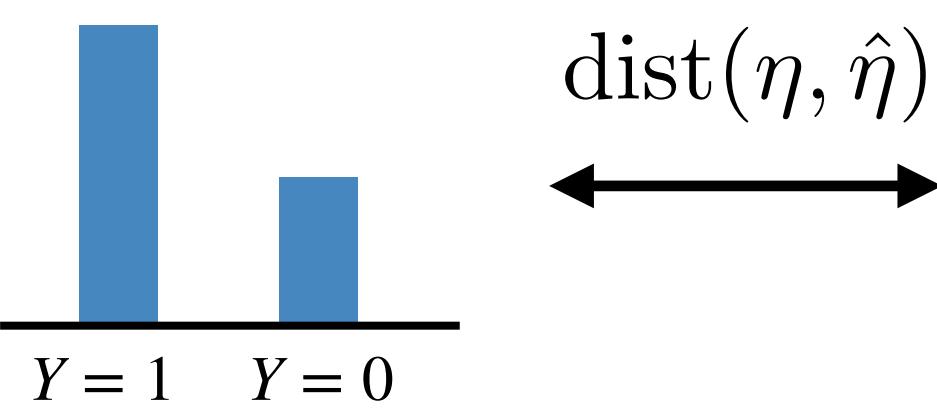
● **Q.** How can estimated probabilities be used for other tasks?

- ❖ Regret bounds

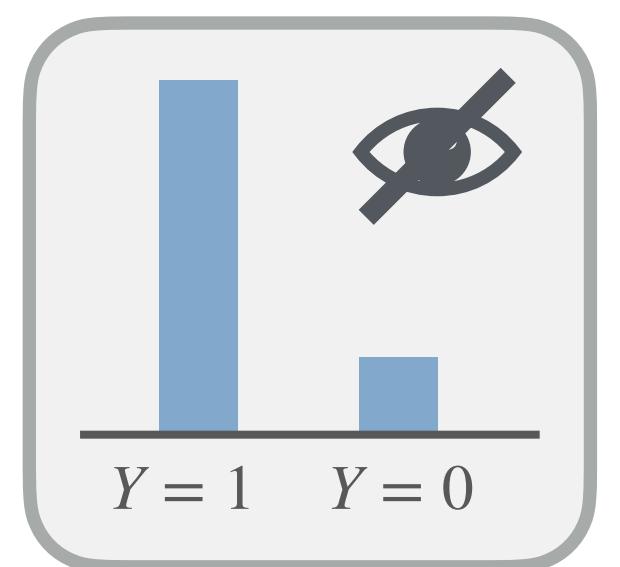
● **Q.** How to compare different loss functions?

- ❖ Order function of moduli

**Proper Losses, Moduli of Convexity,
and Surrogate Regret Bounds**

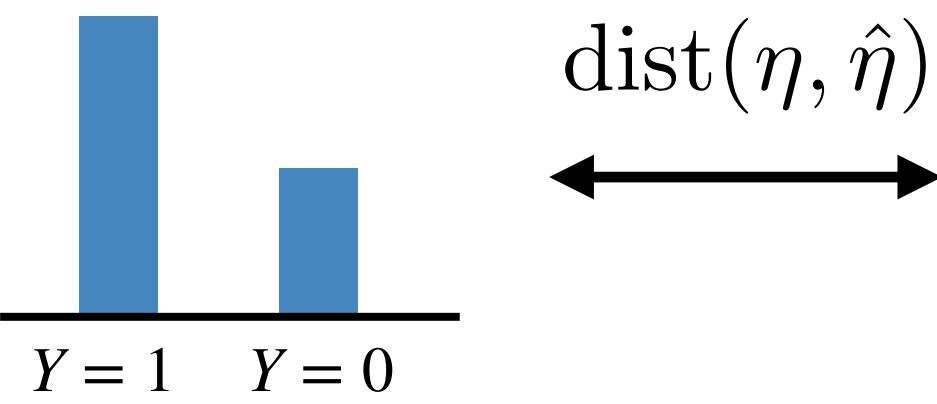


Estimate $\hat{\eta}$

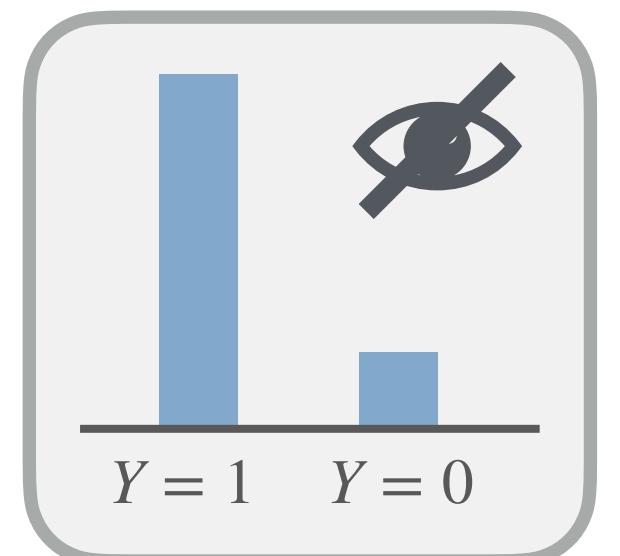


Proper losses

- How to compute $\text{dist}(\eta(\mathbf{x}), \hat{\eta}(\mathbf{x}))$ with only $\hat{\eta}$ and y ?
 - Challenge: no observation of $\eta(\mathbf{x}_i)$



Estimate $\hat{\eta}$



True η

Proper losses

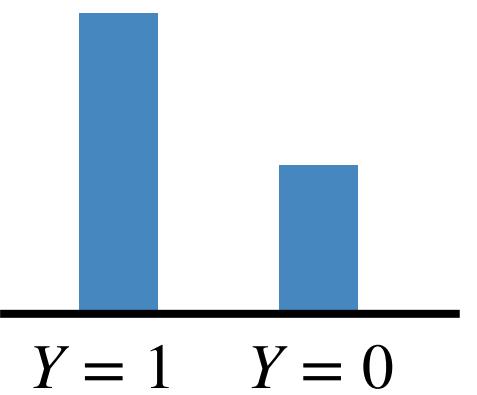
- How to compute $\text{dist}(\eta(\mathbf{x}), \hat{\eta}(\mathbf{x}))$ with only $\hat{\eta}$ and y ?

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- Loss function $\ell(y, \hat{\eta})$

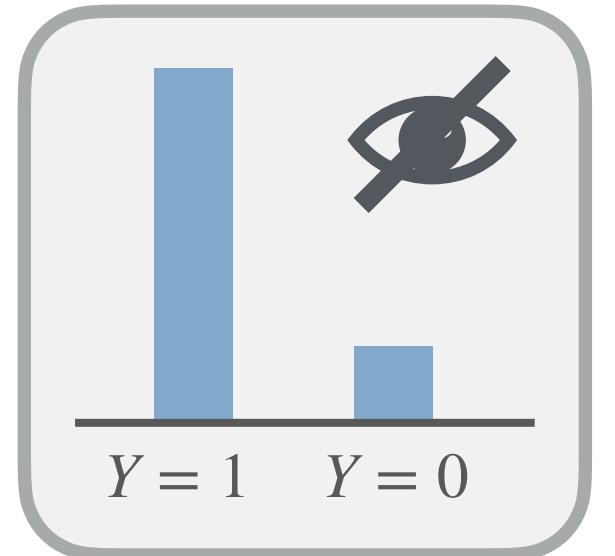
❖ Define loss function for $y \in \{1, 0\}$ separately

❖ Example (log loss): $\ell(y, \hat{\eta}) = \begin{cases} -\ln \hat{\eta} & \text{if } y = 1 \\ -\ln(1 - \hat{\eta}) & \text{if } y = 0 \end{cases}$

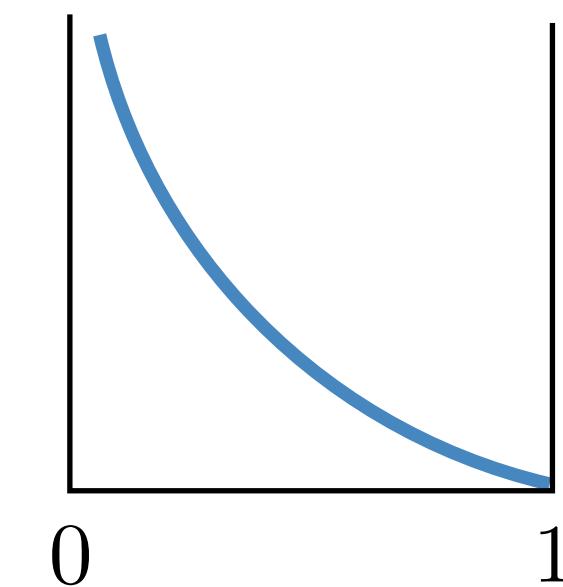


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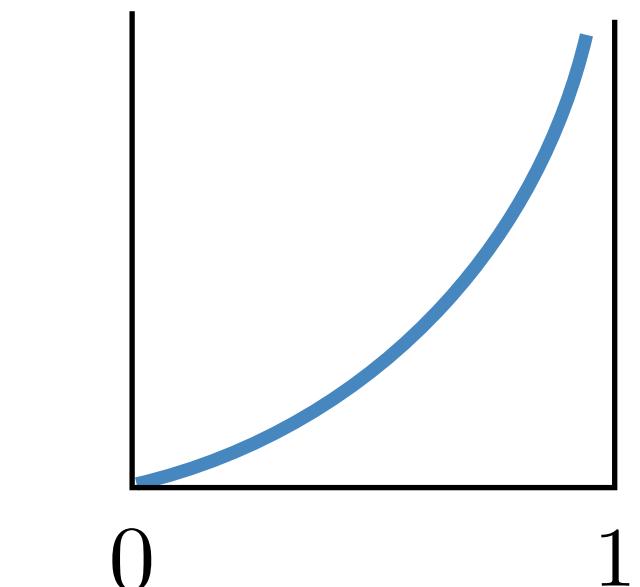
$$\text{dist}(\eta, \hat{\eta})$$



True η



$$\ell(1, \hat{\eta}) = -\ln \hat{\eta}$$



$$\ell(0, \hat{\eta}) = -\ln(1 - \hat{\eta})$$

Proper losses

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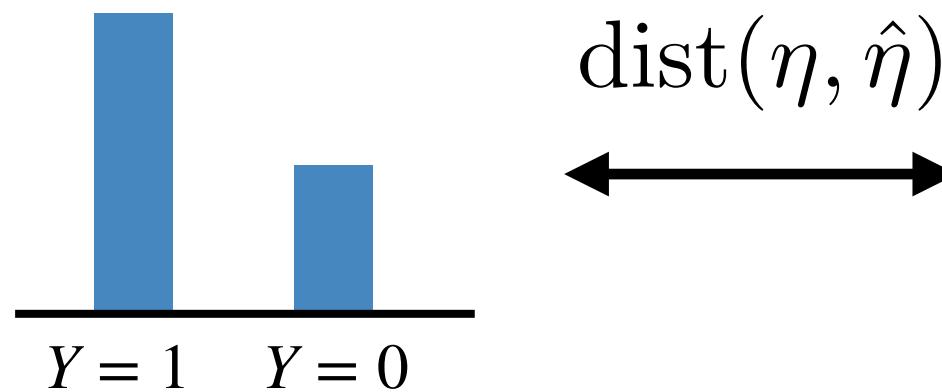
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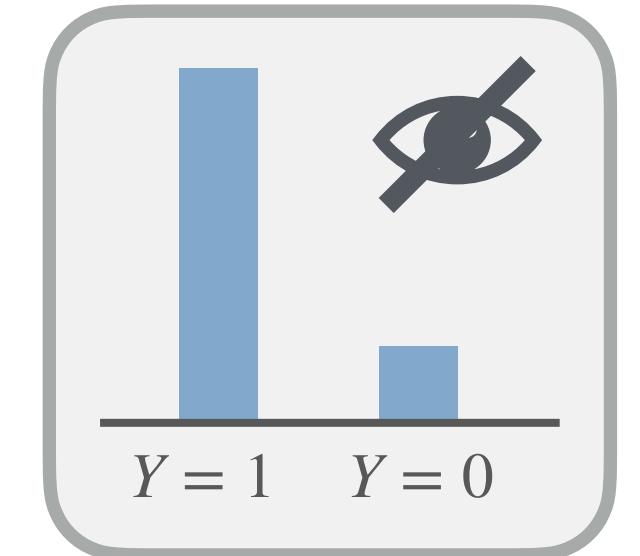
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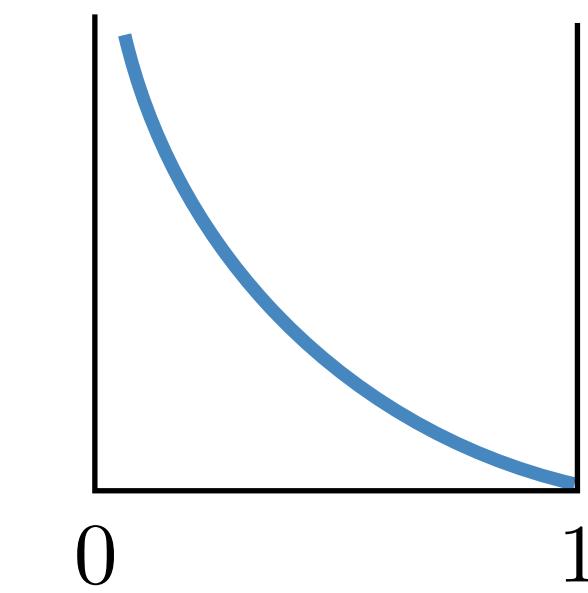
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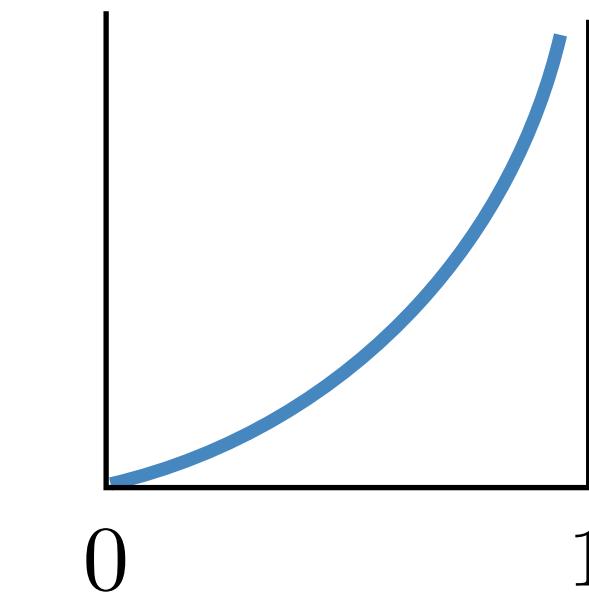
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True η



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Proper losses

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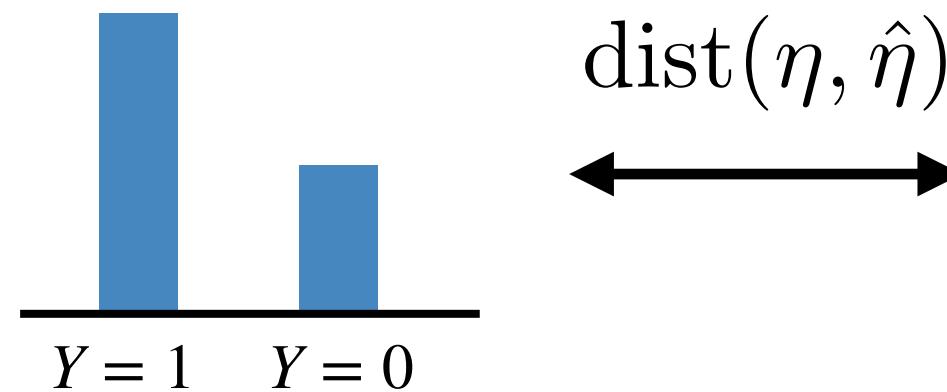
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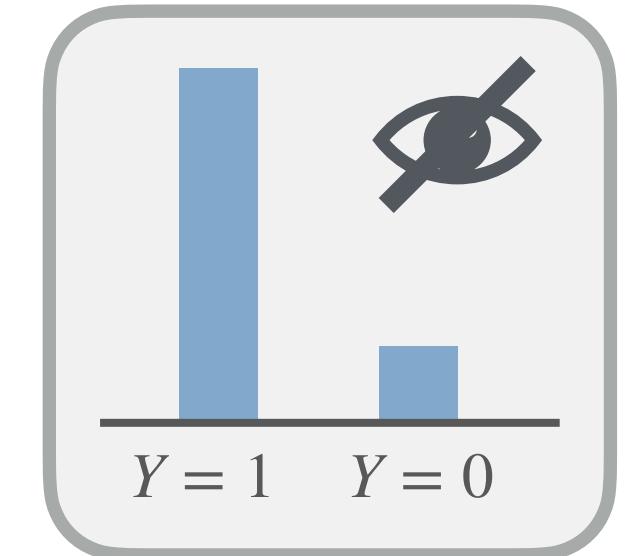
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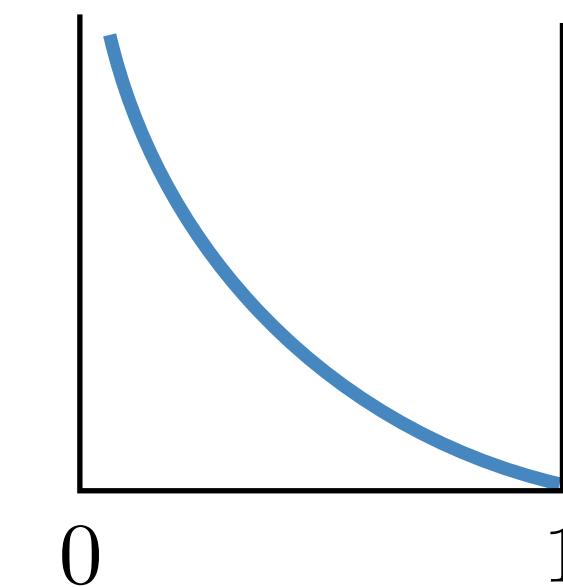
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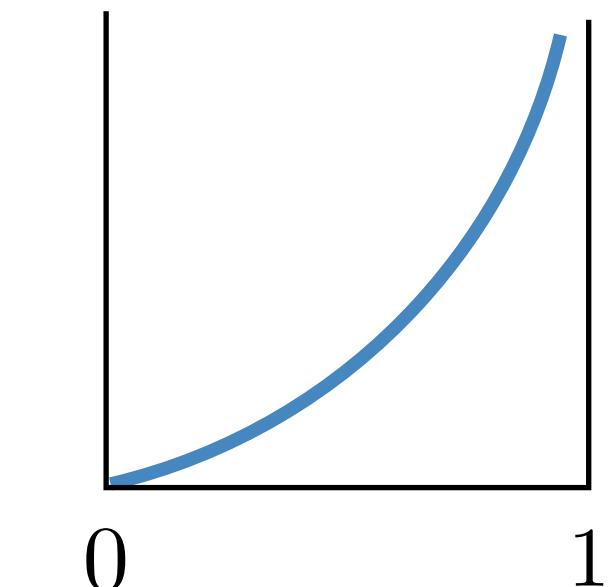
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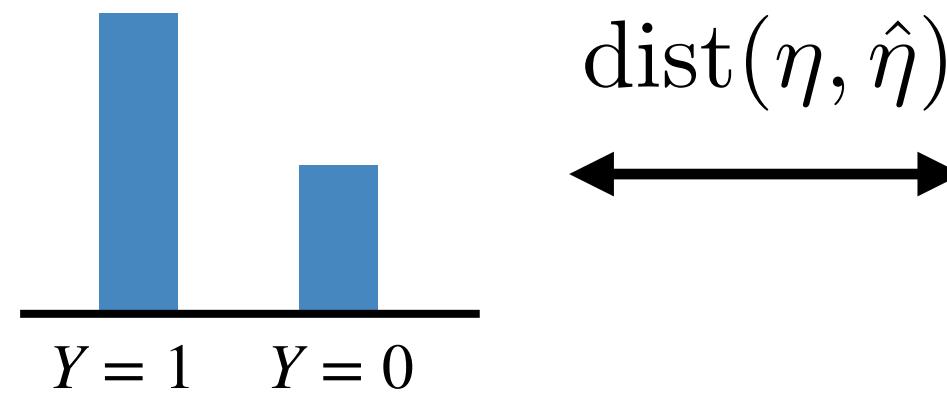
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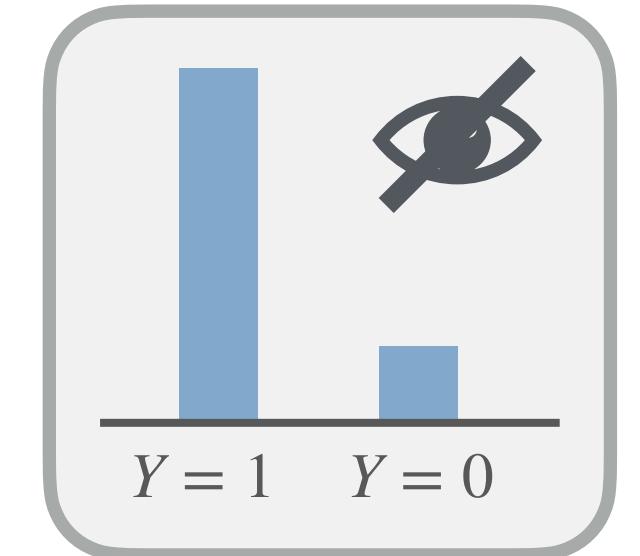
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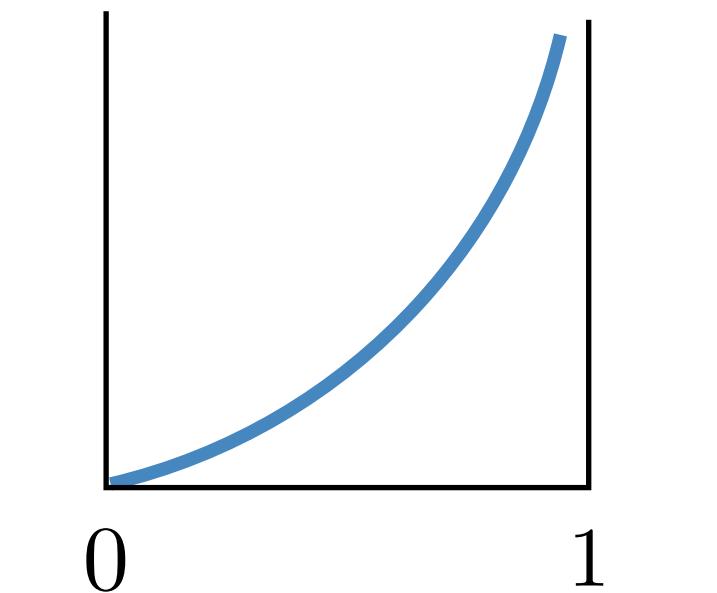
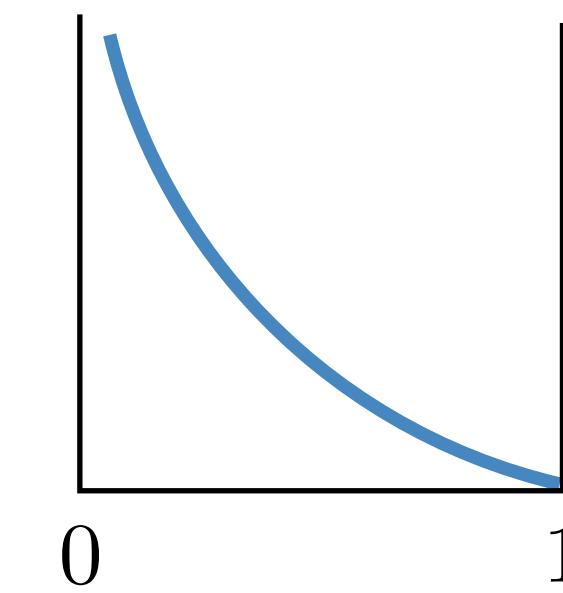
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Estimate $\hat{\eta}$



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 $= \eta\ell(1, \hat{\eta}) + (1 - \eta)\ell(0, \hat{\eta})$
 $= \text{dist}(\eta, \hat{\eta})$
- **Q.** What conditions should $\ell(y, \hat{\eta})$ satisfy?
 - ❖ Minimization of $\text{dist}(\eta, \hat{\eta})$ should lead to $\hat{\eta} \approx \eta$

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Definition [Buja et al., 2005]. $\ell(y, \hat{\eta})$ is proper when $L_\ell(\eta, \eta) = \underline{L}_\ell(\eta)$ for all $\eta \in [0, 1]$.

Conditional risk $L_\ell(\eta, \hat{\eta}) = \eta\ell(1, \hat{\eta}) + (1 - \eta)\ell(0, \hat{\eta})$

Bayes risk $\underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0,1]} L_\ell(\eta, \hat{\eta})$

Proper losses

- dist($\eta(\mathbf{x}), \hat{\eta}(\mathbf{x})$) can be assessed via expected loss $\mathbb{E}_{(X,Y)}\ell(Y, \hat{\eta}(X)) = \mathbb{E}_X [\mathbb{E}_{Y=1|X}\ell(Y, \hat{\eta}(X))]$
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$$\text{Bayes risk } \underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0, 1]} L_\ell(\eta, \hat{\eta})$$

- $\hat{\eta} = \eta$ minimizes conditional risk
- We say $\ell(y, \hat{\eta})$ is strictly proper if the minimizer is unique

Proper losses

- Q. How to test properness?

Theorem [Savage 1971]. ℓ is proper iff \underline{L}_ℓ is concave and

$$L(\eta, \hat{\eta}) = \underline{L}_\ell(\hat{\eta}) + (\eta - \hat{\eta})\underline{L}'_\ell(\hat{\eta}) \text{ for all } \eta, \hat{\eta} \in (0, 1).$$

Theorem [Agarwal 2014]. ℓ is strictly proper iff \underline{L}_ℓ is strictly concave.

Definition. $\ell(y, \hat{\eta})$ is strictly proper iff $L_\ell(\eta, \hat{\eta}) = \underline{L}_\ell(\eta) \iff \hat{\eta} = \eta$ for all $\eta \in [0, 1]$.

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- [⇒] Check strict concavity of \underline{L}_ℓ

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Theorem [Agarwal 2014]. ℓ is strictly proper iff \underline{L}_ℓ is strictly concave.

- [⇒] Check strict concavity of \underline{L}_ℓ
- [⇐] For a concave $H : [0, 1] \rightarrow \mathbb{R}$, loss $\ell(y, \hat{\eta}) = H(\hat{\eta}) + (y - \hat{\eta})H'(\hat{\eta})$ is proper
 - ❖ Remark: proper loss and concave function are closely related

Definition. $\ell(y, \hat{\eta})$ is strictly proper iff $L_\ell(\eta, \hat{\eta}) = \underline{L}_\ell(\eta) \iff \hat{\eta} = \eta$ for all $\eta \in [0, 1]$.

$$L_\ell(\eta, \hat{\eta}) = \eta\ell(1, \hat{\eta}) + (1 - \eta)\ell(0, \hat{\eta}) \quad \underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0, 1]} L_\ell(\eta, \hat{\eta})$$

Examples | log loss

- Log loss $\ell(y, \hat{\eta}) = \begin{cases} -\ln \hat{\eta} & \text{if } y = 1 \\ -\ln(1 - \hat{\eta}) & \text{if } y = 0 \end{cases}$

- Conditional risk** $L_\ell(\eta, \hat{\eta}) = -\eta \ln \hat{\eta} - (1 - \eta) \ln(1 - \hat{\eta})$

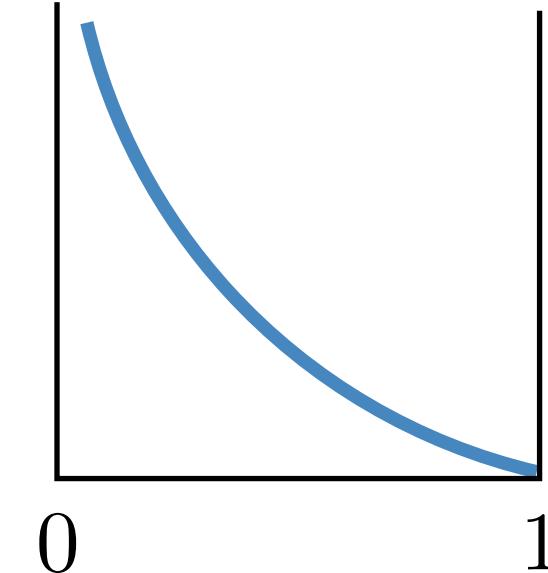
❖ Binary cross-entropy

- Bayes risk** $\underline{L}_\ell(\eta) = -\eta \ln \eta - (1 - \eta) \ln(1 - \eta)$

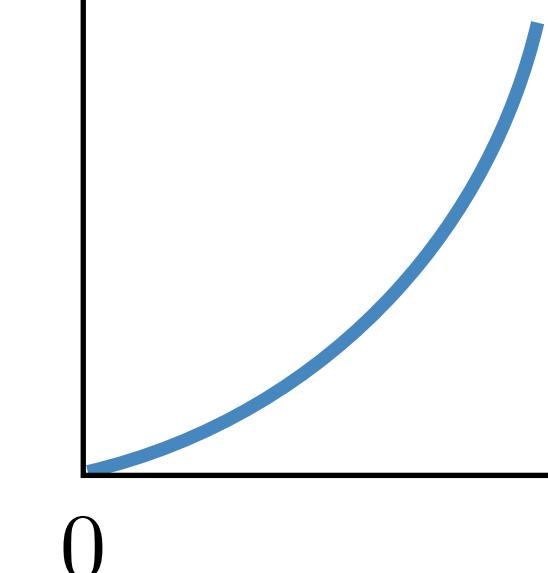
❖ Shannon entropy

- Log loss is strictly proper because Shannon entropy is strictly concave

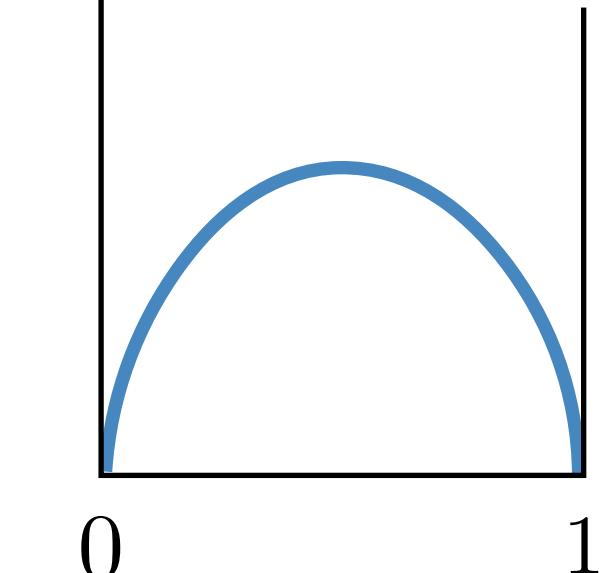
$$\ell(1, \hat{\eta}) = -\ln \hat{\eta}$$



$$\ell(0, \hat{\eta}) = -\ln(1 - \hat{\eta})$$



$$\underline{L}_\ell(\eta)$$



Definition. $\ell(y, \hat{\eta})$ is strictly proper iff $L_\ell(\eta, \hat{\eta}) = \underline{L}_\ell(\eta) \iff \hat{\eta} = \eta$ for all $\eta \in [0, 1]$.

$$L_\ell(\eta, \hat{\eta}) = \eta \ell(1, \hat{\eta}) + (1 - \eta) \ell(0, \hat{\eta})$$

$$\underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0, 1]} L_\ell(\eta, \hat{\eta})$$

Examples | L2 loss

- L2 loss $\ell(y, \hat{\eta}) = \begin{cases} (1 - \hat{\eta})^2 & \text{if } y = 1 \\ \hat{\eta}^2 & \text{if } y = 0 \end{cases}$

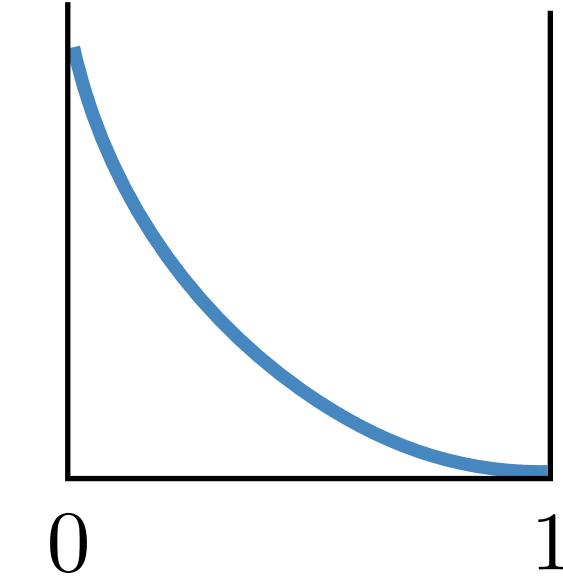
- Conditional risk $L_\ell(\eta, \hat{\eta}) = \eta(1 - \hat{\eta})^2 + (1 - \eta)\hat{\eta}^2$

- Bayes risk $\underline{L}_\ell(\eta) = \eta(1 - \eta)$

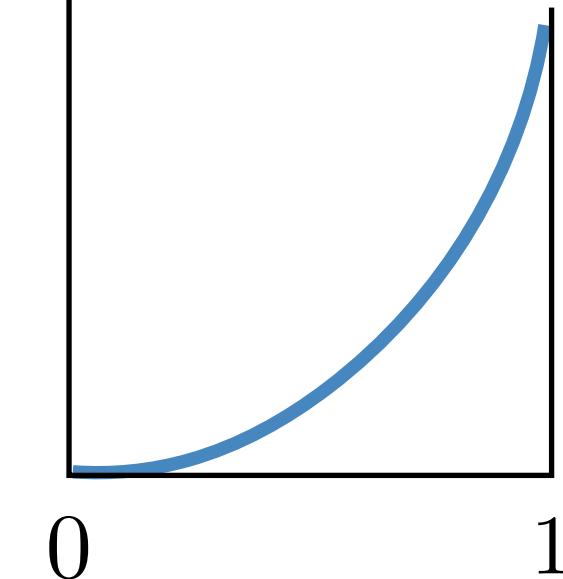
❖ Gini index

- L2 loss is strictly proper because Gini index is strictly concave

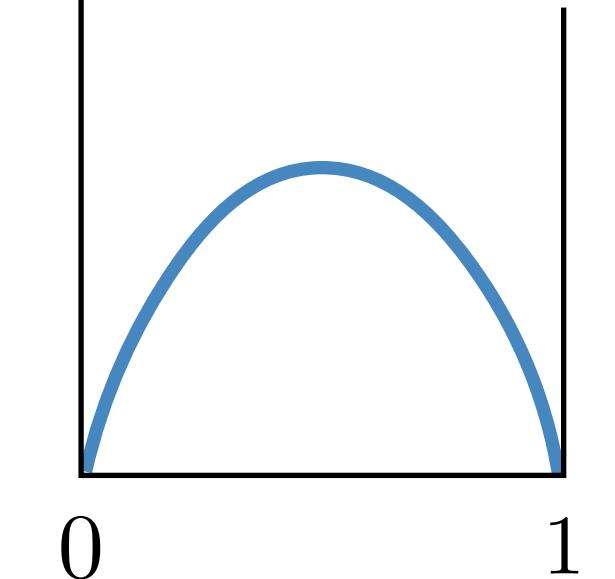
$$\ell(1, \hat{\eta}) = (1 - \hat{\eta})^2$$



$$\ell(0, \hat{\eta}) = \hat{\eta}^2$$



$$\underline{L}_\ell(\eta)$$



Definition. $\ell(y, \hat{\eta})$ is strictly proper iff $L_\ell(\eta, \hat{\eta}) = \underline{L}_\ell(\eta) \iff \hat{\eta} = \eta$ for all $\eta \in [0, 1]$.

$$L_\ell(\eta, \hat{\eta}) = \eta\ell(1, \hat{\eta}) + (1 - \eta)\ell(0, \hat{\eta}) \quad \underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0,1]} L_\ell(\eta, \hat{\eta})$$

Examples | L1 loss

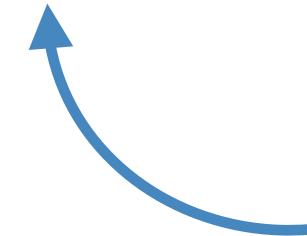
- L1 loss $\ell(y, \hat{\eta}) = \begin{cases} 1 - \hat{\eta} & \text{if } y = 1 \\ \hat{\eta} & \text{if } y = 0 \end{cases}$

- Conditional risk $L_\ell(\eta, \hat{\eta}) = \eta(1 - \hat{\eta}) + (1 - \eta)\hat{\eta}$

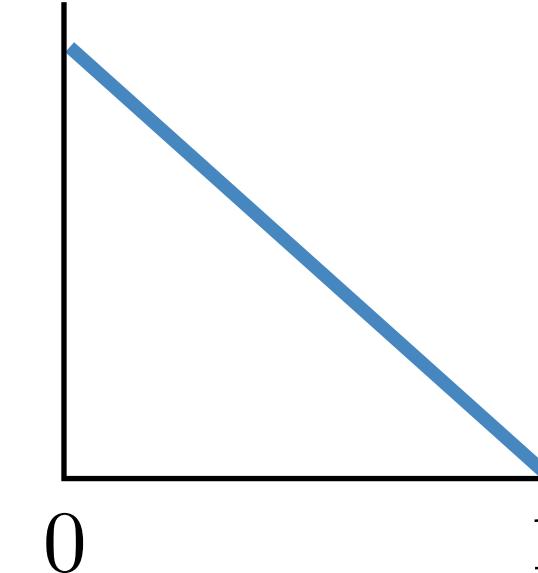
- Bayes risk $\underline{L}_\ell(\eta) = \max\{\eta, 1 - \eta\}$

- L1 loss is not strictly proper **nor proper**

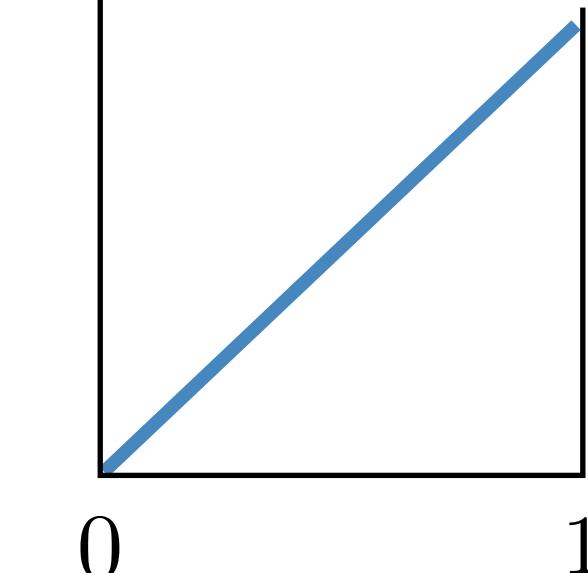
$(\underline{L}_\ell(\eta)$ is not strictly concave)



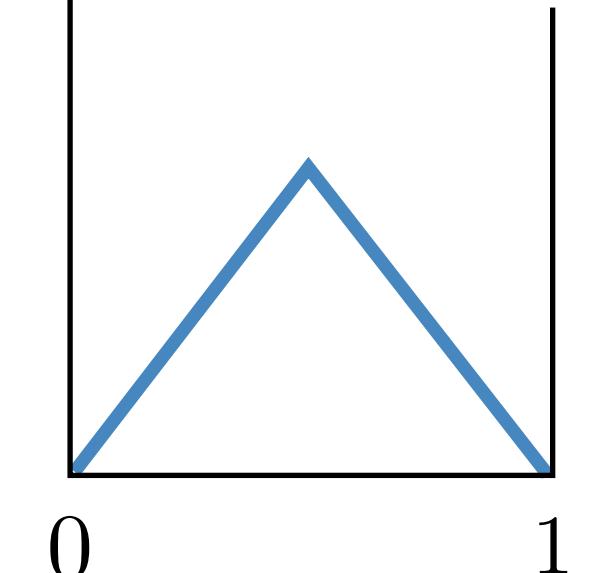
$$\ell(1, \hat{\eta}) = 1 - \hat{\eta}$$



$$\ell(0, \hat{\eta}) = \hat{\eta}$$



$$\underline{L}_\ell(\eta)$$



Theorem. ℓ is proper iff \underline{L}_ℓ is concave and $L(\eta, \hat{\eta}) = \underline{L}_\ell(\hat{\eta}) + (\eta - \hat{\eta})\underline{L}'_\ell(\hat{\eta})$.

Theorem. ℓ is strictly proper iff \underline{L}_ℓ is strictly concave.

$$L(\eta, \hat{\eta}) \neq \underline{L}_\ell(\hat{\eta}) + (\eta - \hat{\eta})\underline{L}'_\ell(\hat{\eta}) = \begin{cases} \eta & \text{if } \hat{\eta} \in [0, \frac{1}{2}] \\ 1 - \eta & \text{if } \hat{\eta} \in (\frac{1}{2}, 1] \end{cases}$$

Outline

- **Q.** How should we assess probability estimates?

- ❖ Proper losses

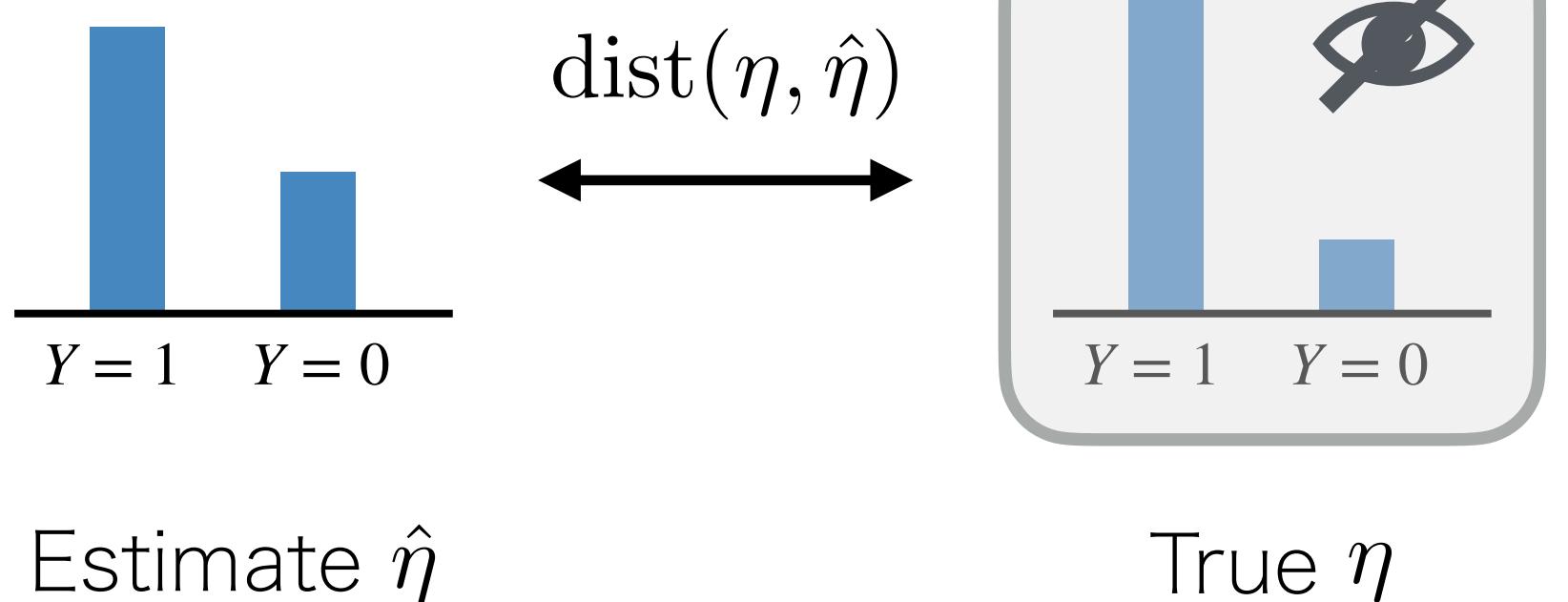
- **Q.** How can estimated probabilities be used for other tasks?

- ❖ Regret bounds

- **Q.** How to compare different loss functions?

- ❖ Order function of moduli

Proper Losses, Moduli of Convexity, and Surrogate Regret Bounds



Proper loss vs. downstream tasks?

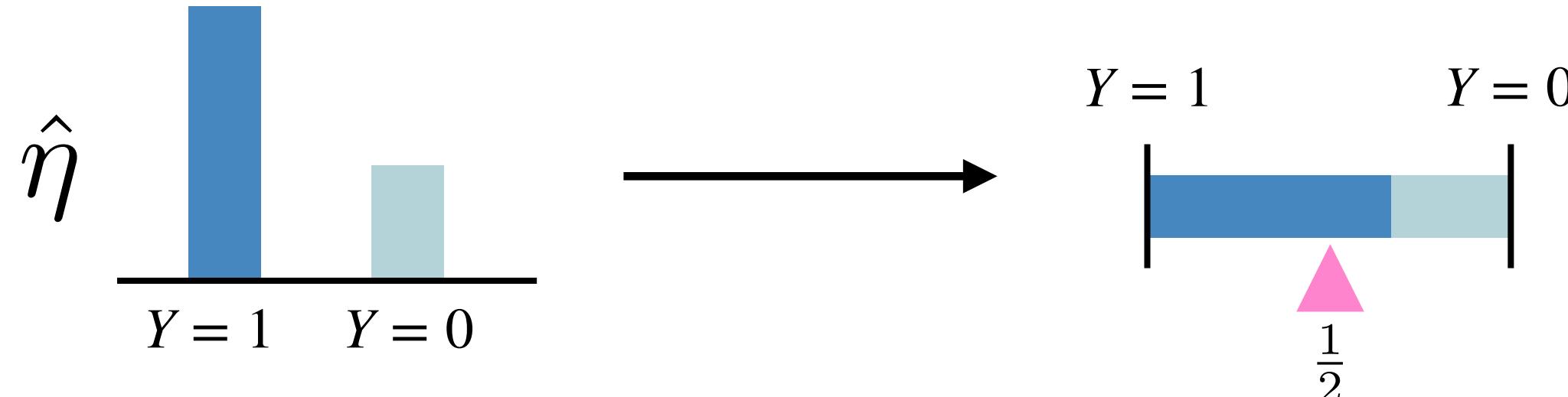
- Formulation of probability estimation: $\min_{\hat{\eta}: \mathcal{X} \rightarrow [0,1]} \mathbb{E}_X [L_\ell(\eta(X), \hat{\eta}(X))]$

❖ We focus on “pointwise” problem $\min_{\hat{\eta} \in [0,1]} L_\ell(\eta, \hat{\eta})$

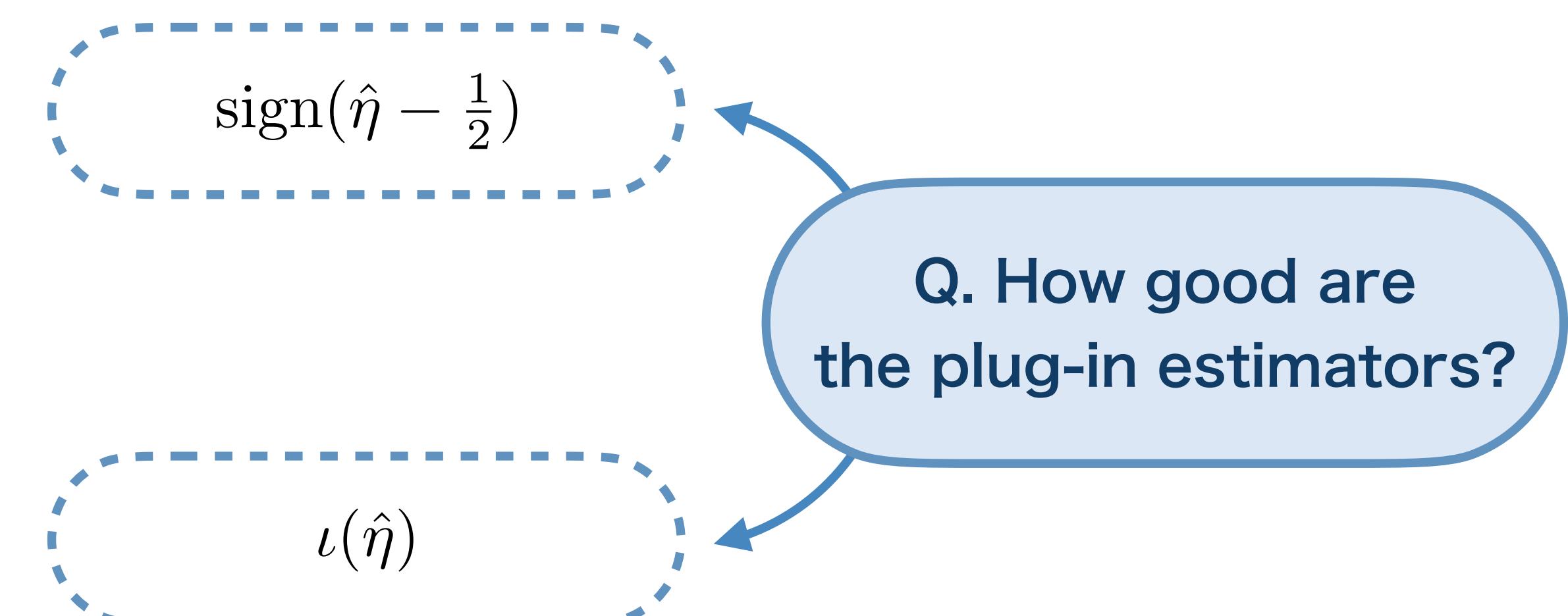
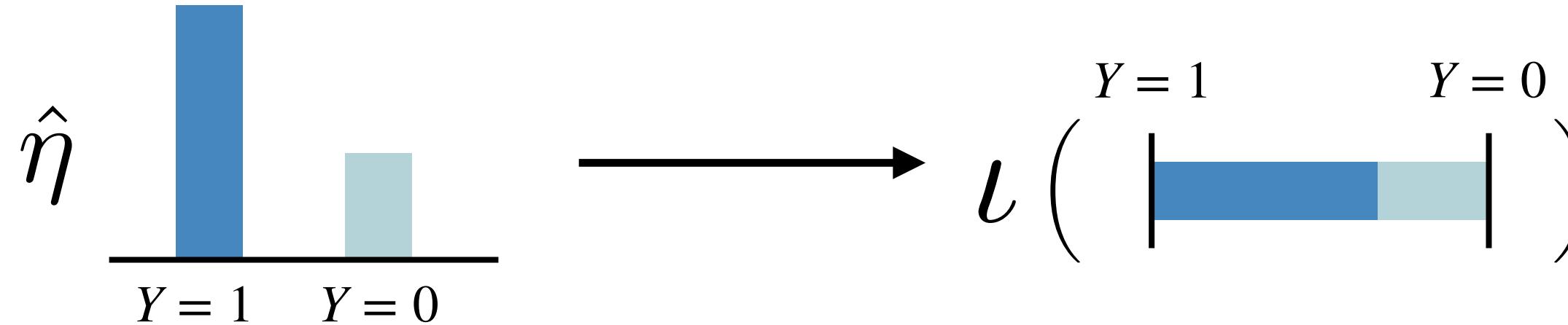
❖ Equivalent to minimizing **regret** $R_\ell(\eta, \hat{\eta}) = L_\ell(\eta, \hat{\eta}) - \underline{L}_\ell(\eta)$

- Q.** How much does estimated $\hat{\eta}$ perform well for downstream tasks?

❖ Classification



❖ Ranking



How to relate a proper loss with downstream tasks?

Our attempt: to derive **L1 regret bound**

$$|\eta - \hat{\eta}| \leq \psi(R_\ell(\eta, \hat{\eta})) \text{ for regret } R_\ell(\eta, \hat{\eta}) = L_\ell(\eta, \hat{\eta}) - \underline{L}_\ell(\eta)$$

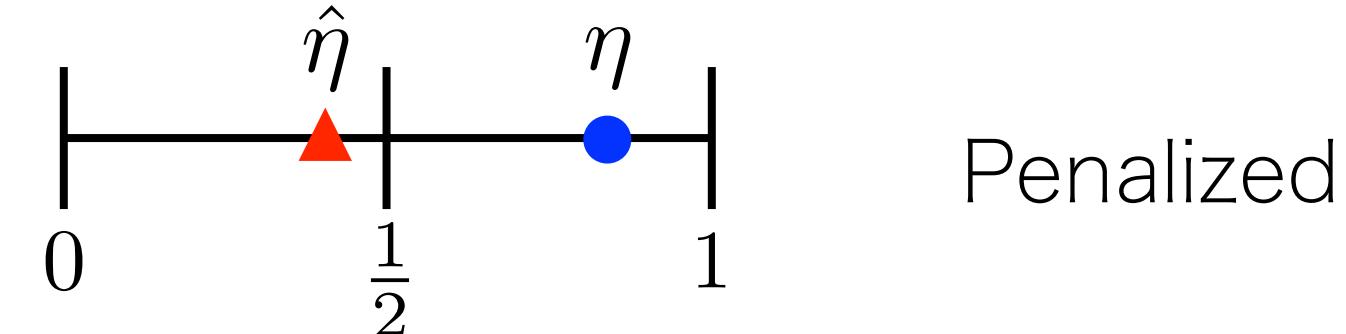
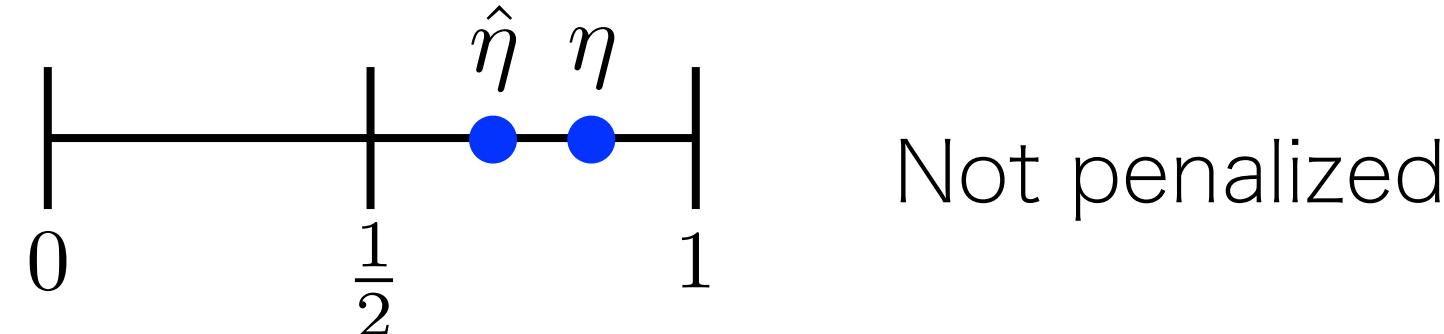
- Why? Because the optimality of downstream tasks can be bounded by $|\eta - \hat{\eta}|$

How to relate a proper loss with downstream tasks?

Out attempt: to derive **L1 regret bound**

$$|\eta - \hat{\eta}| \leq \psi(R_\ell(\eta, \hat{\eta})) \text{ for regret } R_\ell(\eta, \hat{\eta}) = L_\ell(\eta, \hat{\eta}) - \underline{L}_\ell(\eta)$$

- Why? Because the optimality of downstream tasks can be bounded by $|\eta - \hat{\eta}|$
- Classification $R_{01}(\eta, \hat{\eta}) = |\eta - \frac{1}{2}| \llbracket \min\{\eta, \hat{\eta}\} \leq \frac{1}{2} < \max\{\eta, \hat{\eta}\} \rrbracket \leq |\eta - \hat{\eta}|$ [Menon et al., 2013]

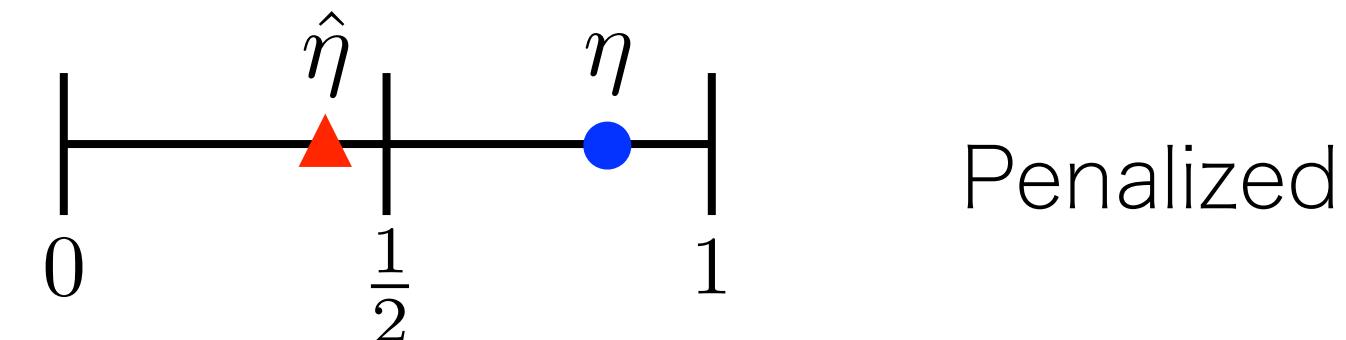
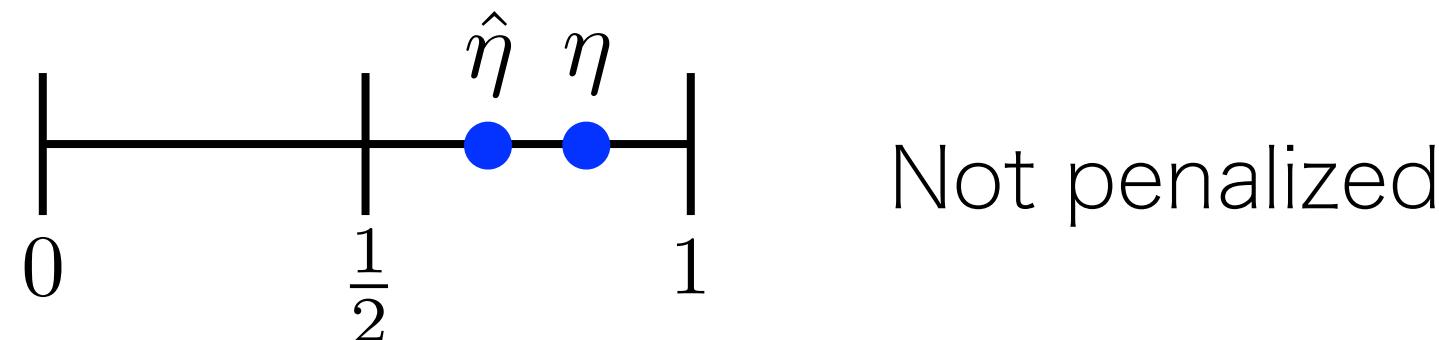


How to relate a proper loss with downstream tasks?

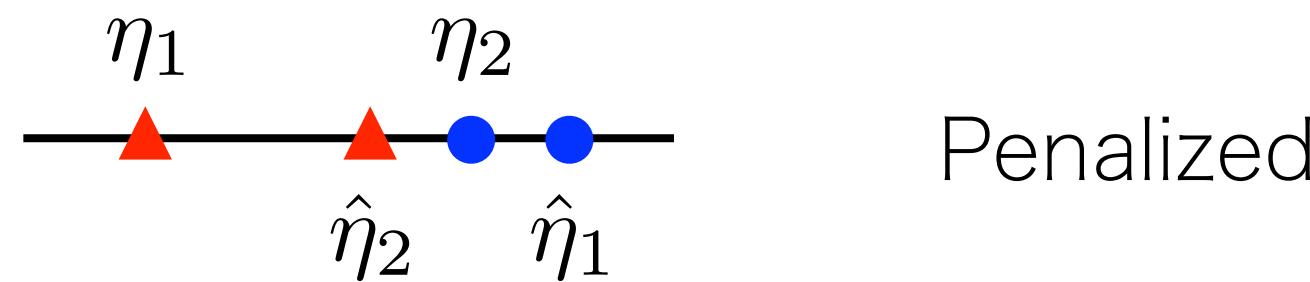
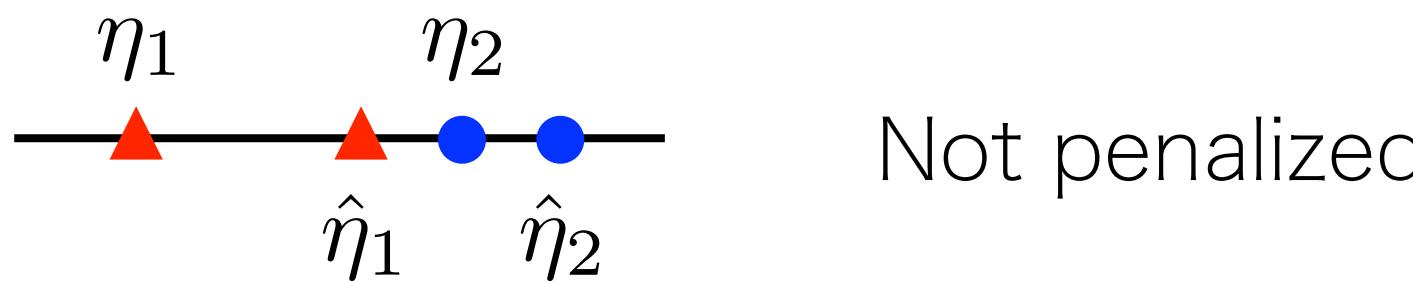
Our attempt: to derive **L1 regret bound**

$$|\eta - \hat{\eta}| \leq \psi(R_\ell(\eta, \hat{\eta})) \text{ for regret } R_\ell(\eta, \hat{\eta}) = L_\ell(\eta, \hat{\eta}) - \underline{L}_\ell(\eta)$$

- Why? Because the optimality of downstream tasks can be bounded by $|\eta - \hat{\eta}|$
- Classification $R_{01}(\eta, \hat{\eta}) = |\eta - \frac{1}{2}| \llbracket \min\{\eta, \hat{\eta}\} \leq \frac{1}{2} < \max\{\eta, \hat{\eta}\} \rrbracket \leq |\eta - \hat{\eta}|$ [Menon et al., 2013]



- Ranking $R_{\text{rank}}(\eta_1, \eta_2, \hat{\eta}_1, \hat{\eta}_2) = |\eta_1 - \eta_2| \llbracket (\hat{\eta}_1 - \hat{\eta}_2)(\eta_1 - \eta_2) < 0 \rrbracket \leq |\eta_1 - \hat{\eta}_1| + |\eta_2 - \hat{\eta}_2|$ [Agarwal 2014]



Motivation of our work

Our attempt: to derive **L1 regret bound**

$$|\eta - \hat{\eta}| \leq \psi(R_\ell(\eta, \hat{\eta})) \text{ for regret } R_\ell(\eta, \hat{\eta}) = L_\ell(\eta, \hat{\eta}) - \underline{L}_\ell(\eta)$$

- Regret bound reads:
minimizing regret R_ℓ amounts to be optimizing downstream performance via $|\eta - \hat{\eta}|$
- Motivation 1: to avoid deriving regret bounds for each task independently
- Motivation 2: to get more insight into relationship between a proper loss and ψ
- Consequently, we ask
 - ❖ Any loss performs universally well for various tasks?
 - ❖ Which loss entails faster rate?

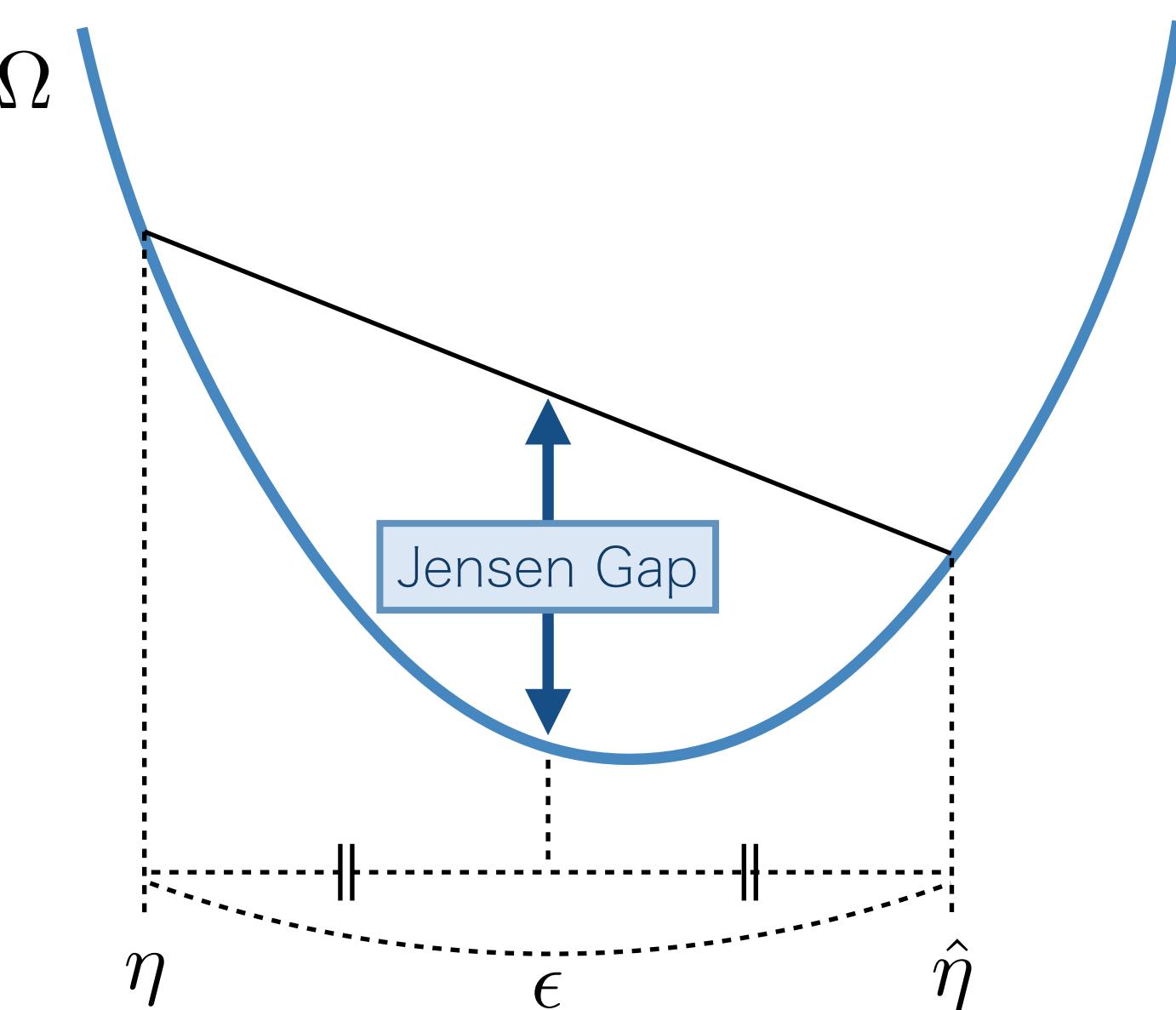
Preparation | Moduli of convexity

Definition. For a convex function $\Omega : [0, 1] \rightarrow \mathbb{R}$, its modulus of convexity is

$$\delta_\Omega(\epsilon) := \inf_{\eta, \hat{\eta} \in [0, 1]} \left\{ \frac{\Omega(\eta) + \Omega(\hat{\eta})}{2} - \Omega\left(\frac{\eta + \hat{\eta}}{2}\right) \mid |\eta - \hat{\eta}| \geq \epsilon \right\}.$$

- Moduli = the minimum Jensen gap of a convex function

- ❖ Ω is strictly convex iff $\delta_\Omega(\epsilon) > 0 \quad \forall \epsilon > 0$
- ❖ Generalization of strongly convex functions with $\delta_\Omega(\epsilon) = \frac{\mu}{2}\epsilon^2$



Main theorem | Regret upper bounds

Theorem. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, for all $\eta, \hat{\eta} \in [0, 1]$,

$$\delta_{-\underline{L}_\ell}(|\eta - \hat{\eta}|) \leq R_\ell(\eta, \hat{\eta}).$$

- Monotone function $\delta_{-\underline{L}_\ell}$ governs L1 regret bound ($-\underline{L}_\ell$: convex)

- Corollary.** Regret bounds for downstream tasks

❖ Classification $R_{01}(\eta, \hat{\eta}) \leq (\delta_{-\underline{L}_\ell}^{**})^{-1}(R_\ell(\eta, \hat{\eta}))$

❖ Ranking $R_{\text{rank}}(\eta_1, \eta_2, \hat{\eta}_1, \hat{\eta}_2) \leq (\delta_{-\underline{L}_\ell}^{**})^{-1}(R_\ell(\eta_1, \hat{\eta}_1)) + (\delta_{-\underline{L}_\ell}^{**})^{-1}(R_\ell(\eta_2, \hat{\eta}_2))$
 $(\delta_\Omega^{**} \text{ is convex biconjugate, and hence convex})$

Regret $R_\ell(\eta, \hat{\eta}) = L_\ell(\eta, \hat{\eta}) - \underline{L}_\ell(\eta)$

Conditional risk $L_\ell(\eta, \hat{\eta}) = \eta\ell(1, \hat{\eta}) + (1 - \eta)\ell(0, \hat{\eta})$

Bayes risk $\underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0, 1]} L_\ell(\eta, \hat{\eta})$

Proof sketch

Theorem. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, for all $\eta, \hat{\eta} \in [0, 1]$,

$$\delta_{-\underline{L}_\ell}(|\eta - \hat{\eta}|) \leq R_\ell(\eta, \hat{\eta}).$$

- Modulus is bounded by **Jensen-Bregman divergence**

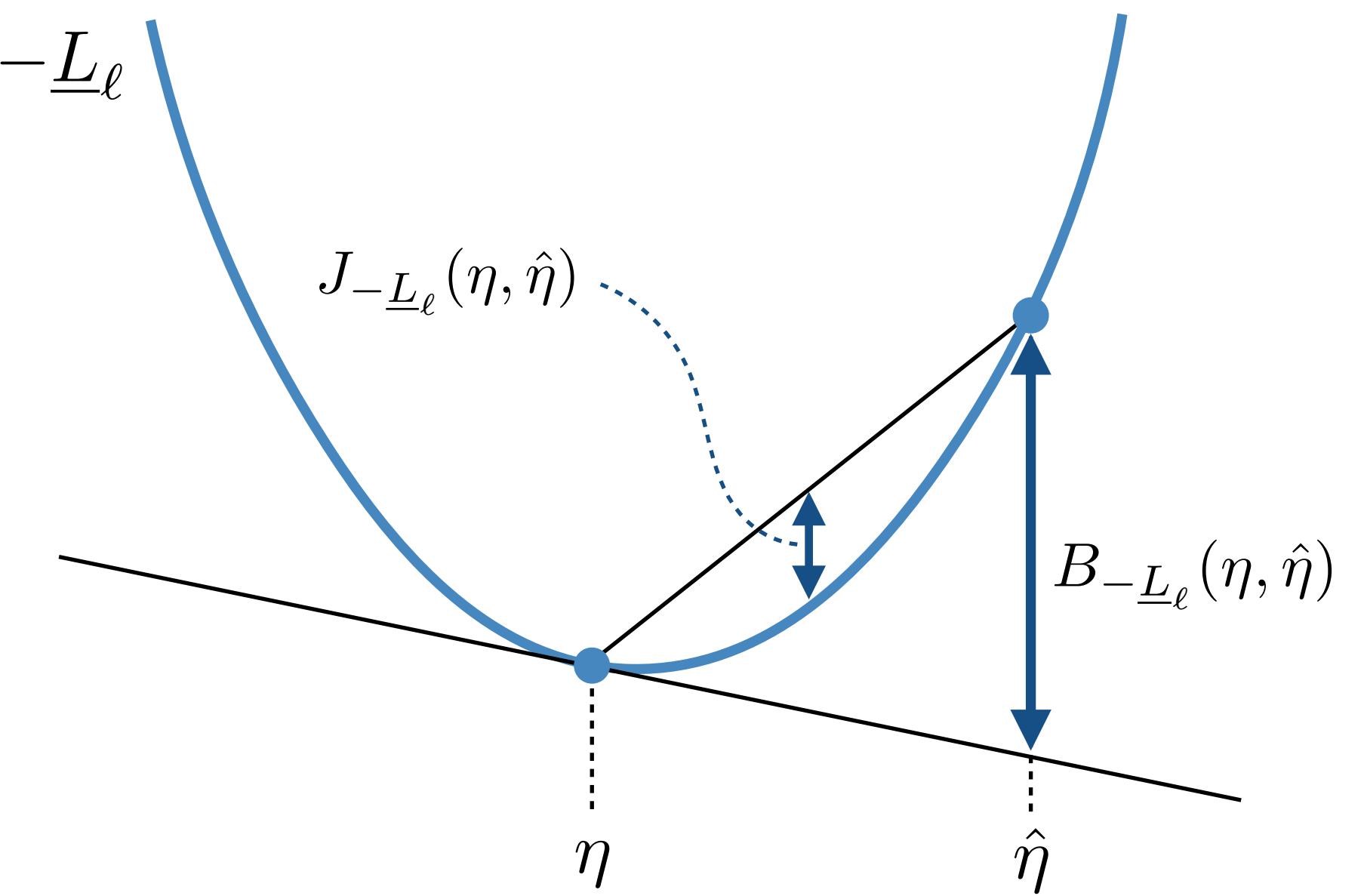
$$\delta_{-\underline{L}_\ell}(\epsilon) \leq \frac{-\underline{L}_\ell(\eta) - \underline{L}_\ell(\hat{\eta})}{2} + \underline{L}_\ell\left(\frac{\eta + \hat{\eta}}{2}\right) =: J_{-\underline{L}_\ell}(\eta, \hat{\eta})$$

- Regret of proper loss = **Bregman divergence**

$$R_\ell(\eta, \hat{\eta}) = -\underline{L}_\ell(\hat{\eta}) + \underline{L}_\ell(\eta) + (\hat{\eta} - \eta)\underline{L}'_\ell(\eta) =: B_{-\underline{L}_\ell}(\eta, \hat{\eta})$$

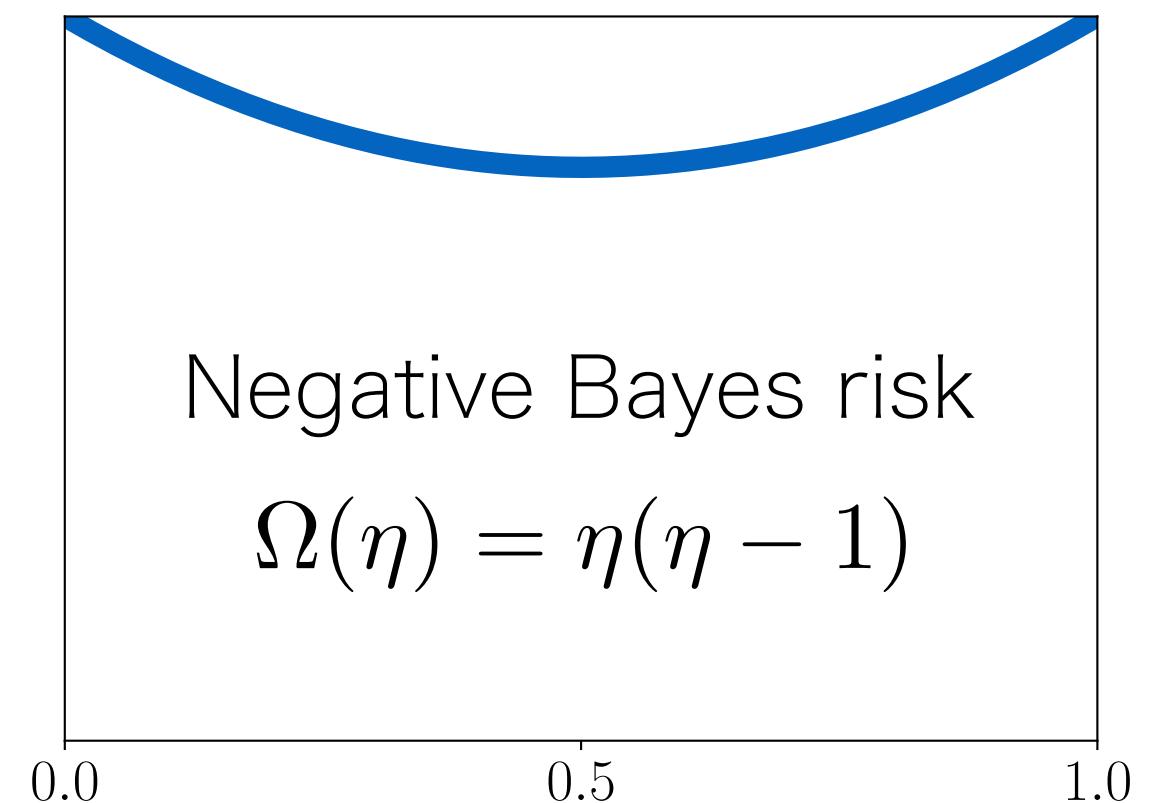
- It is sufficient to show $J_{-\underline{L}_\ell}(\eta, \hat{\eta}) \leq B_{-\underline{L}_\ell}(\eta, \hat{\eta})$

- ❖ Evident from figure



Examples

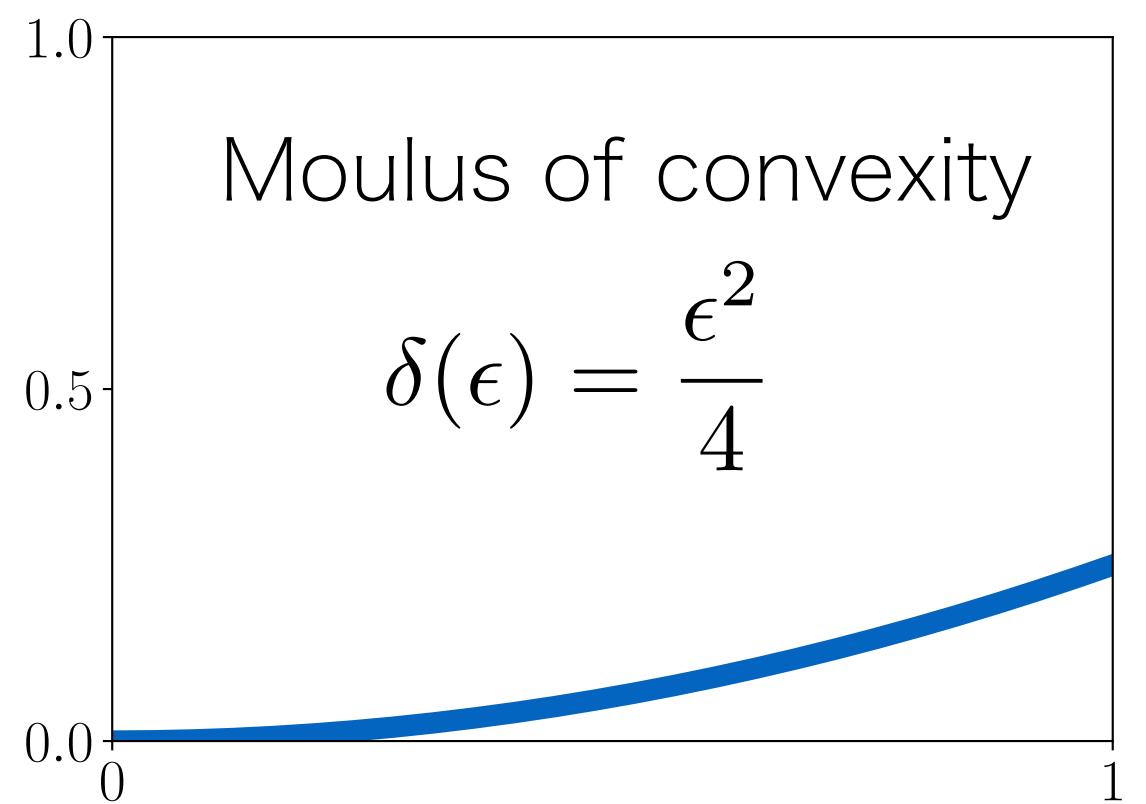
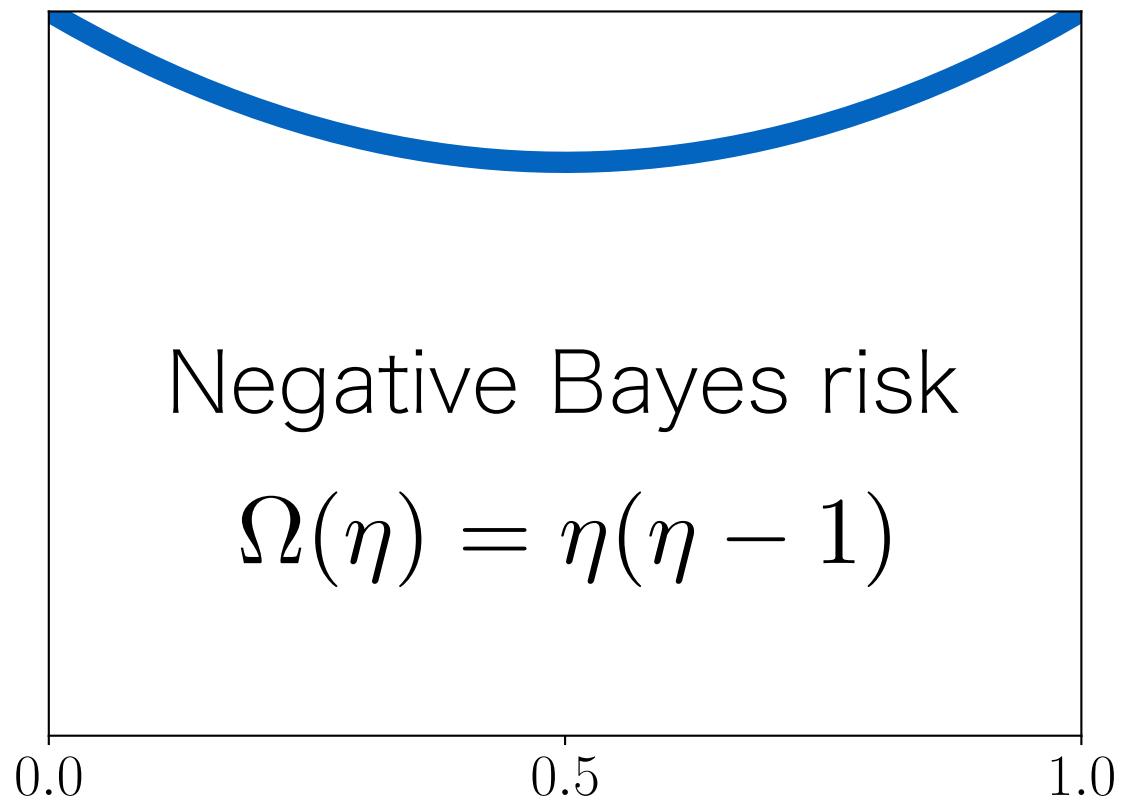
- L2 loss



($\Omega = -\underline{L}_\ell$)

Examples

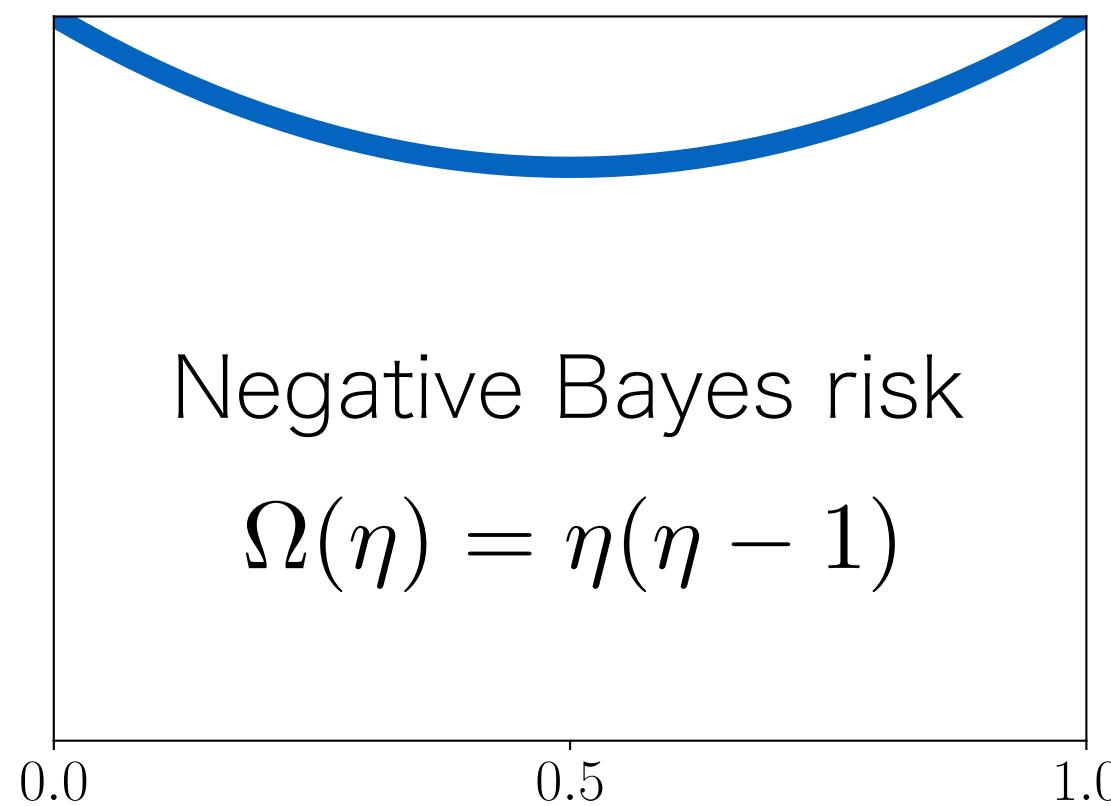
- L2 loss



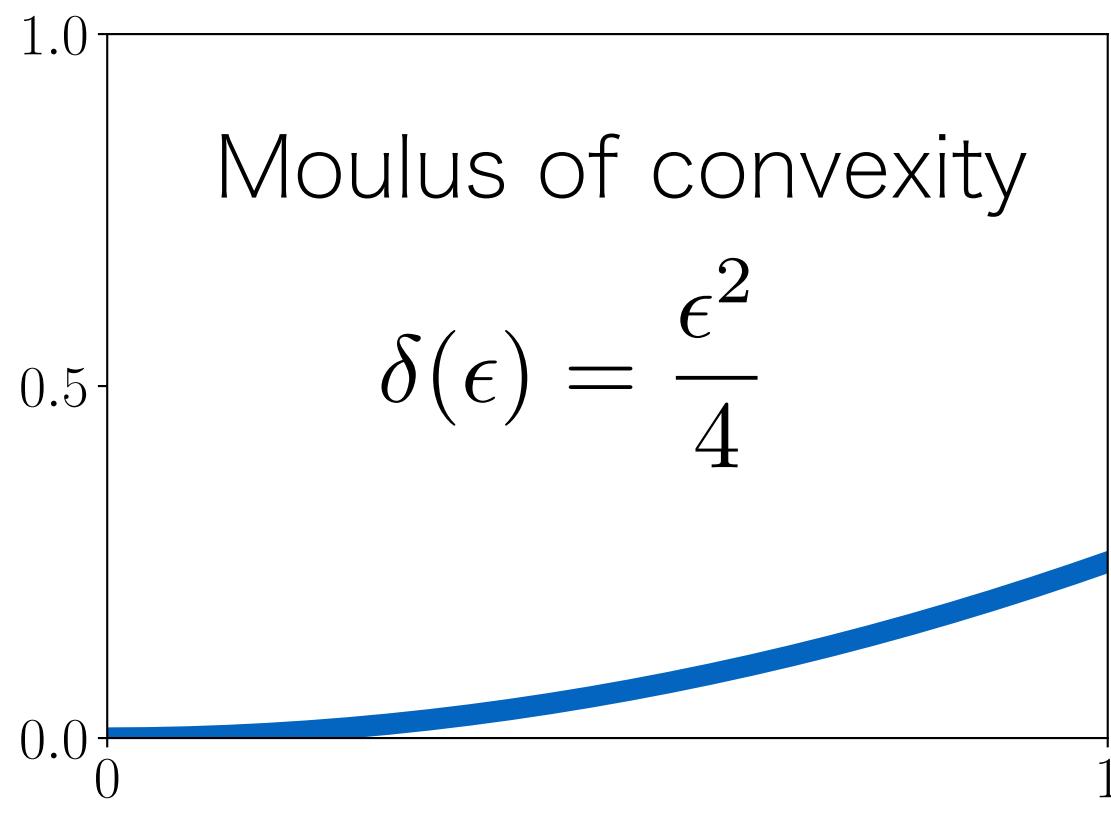
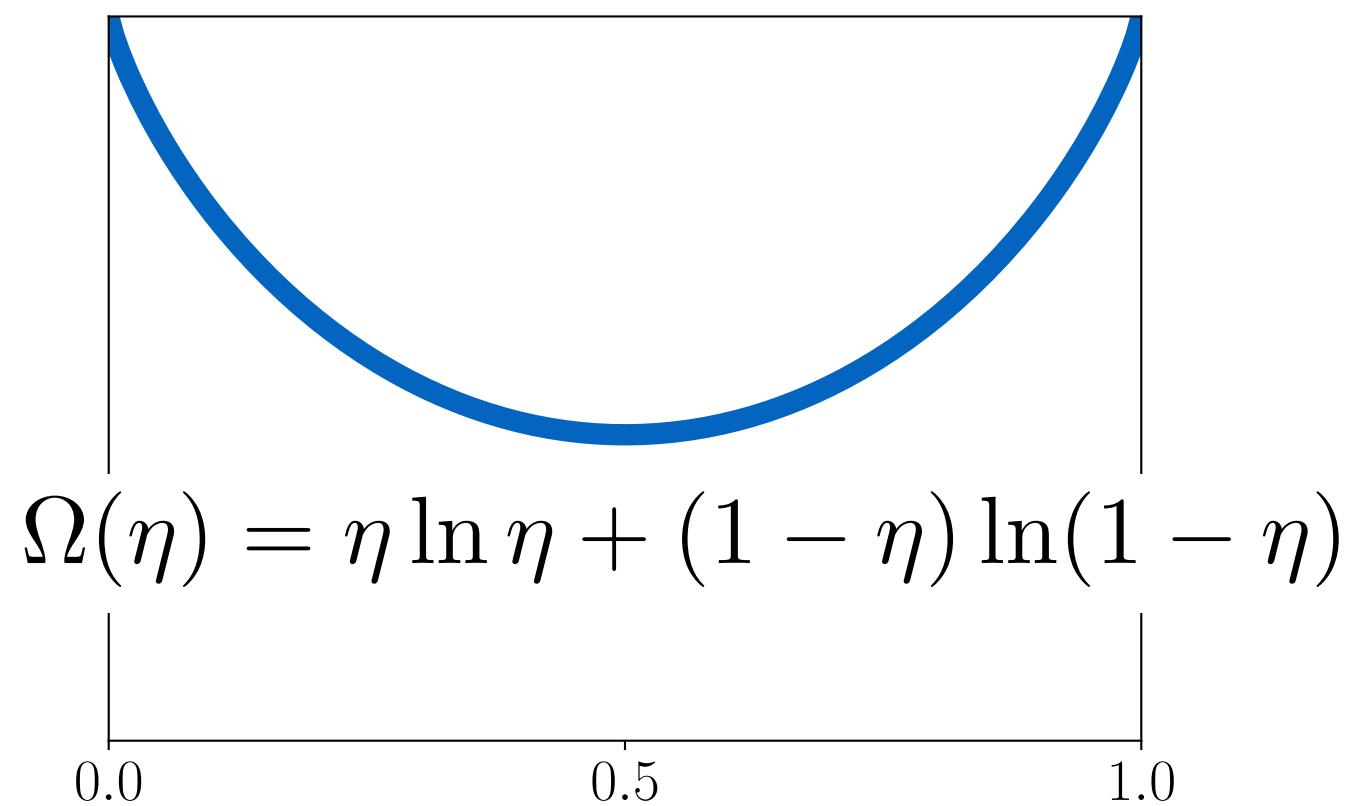
($\Omega = -\underline{L}_\ell$)

Examples

● L2 loss



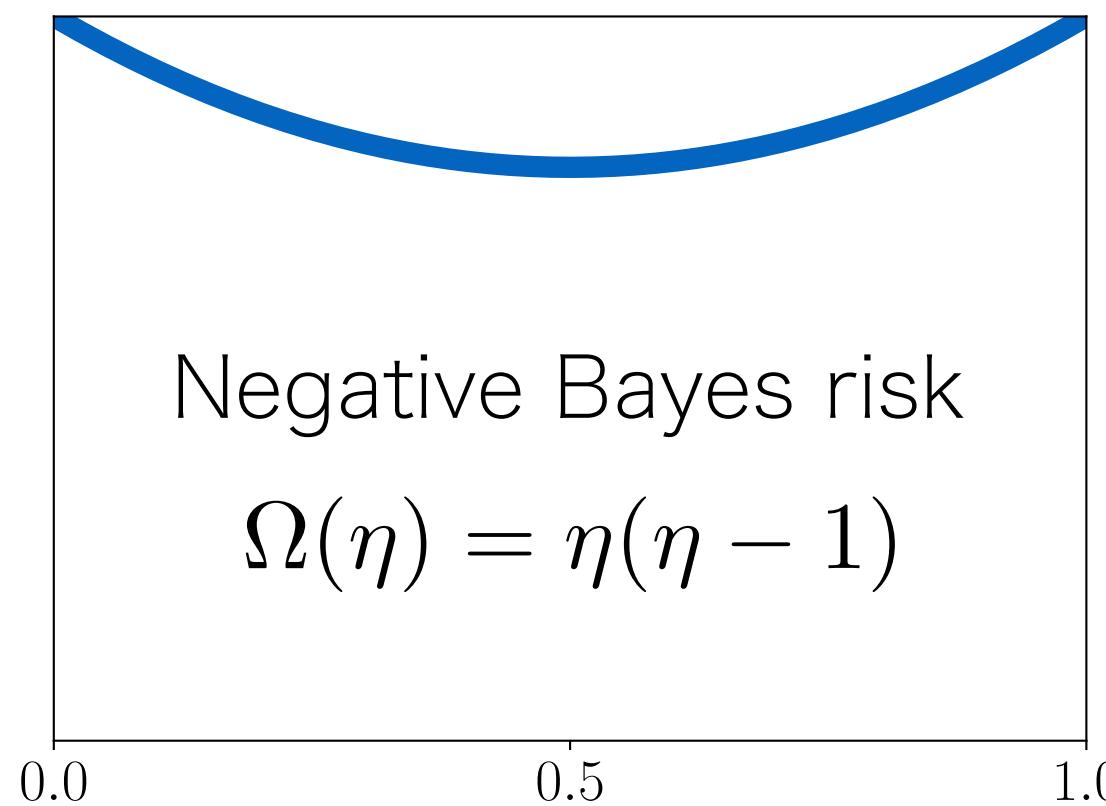
● Log loss



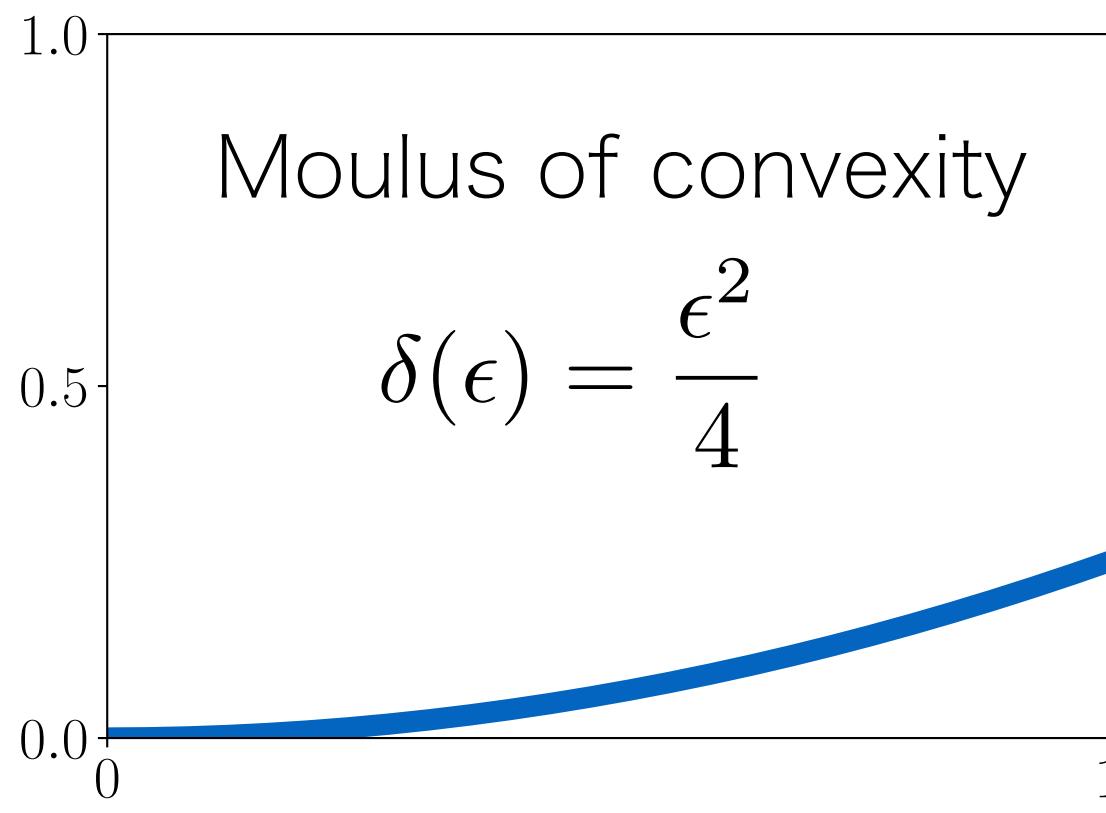
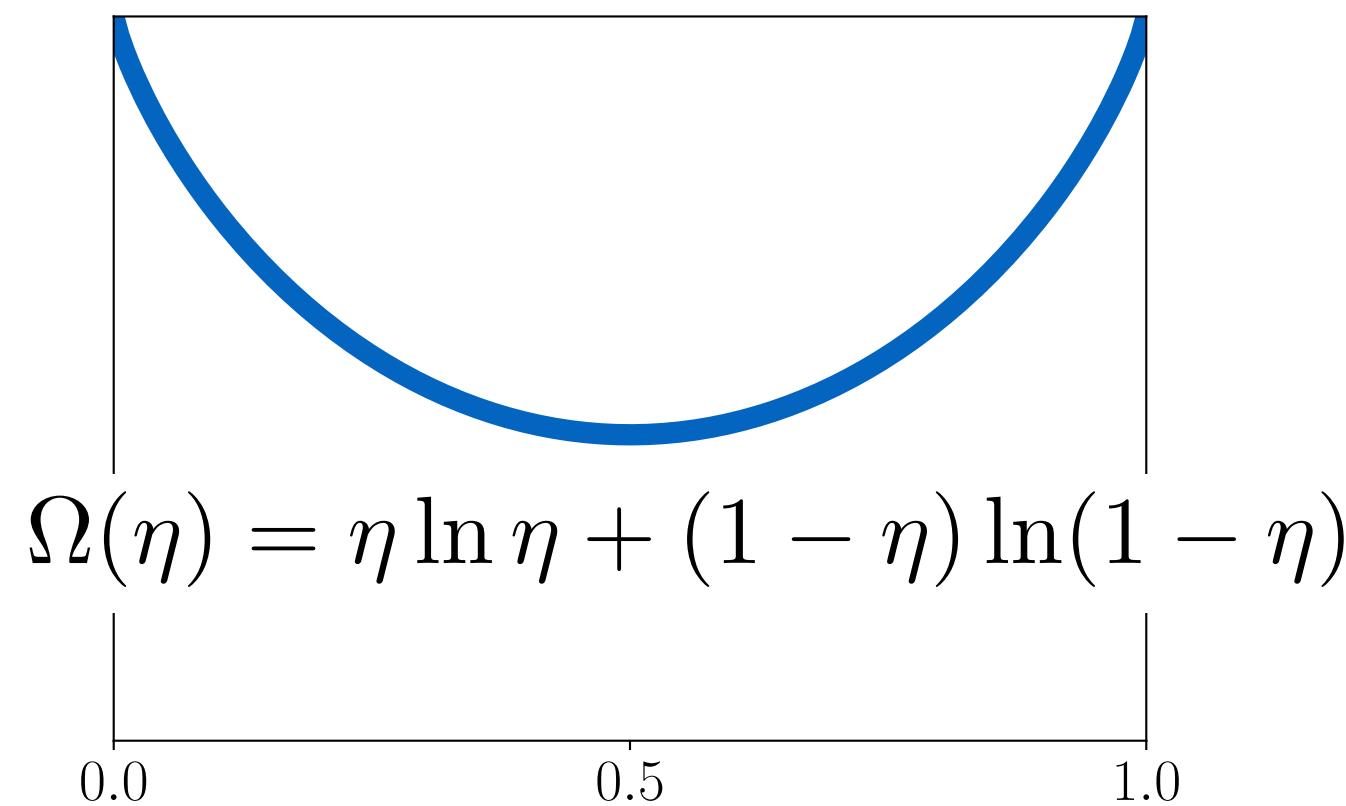
$(\Omega = -\underline{L}_\ell)$

Examples

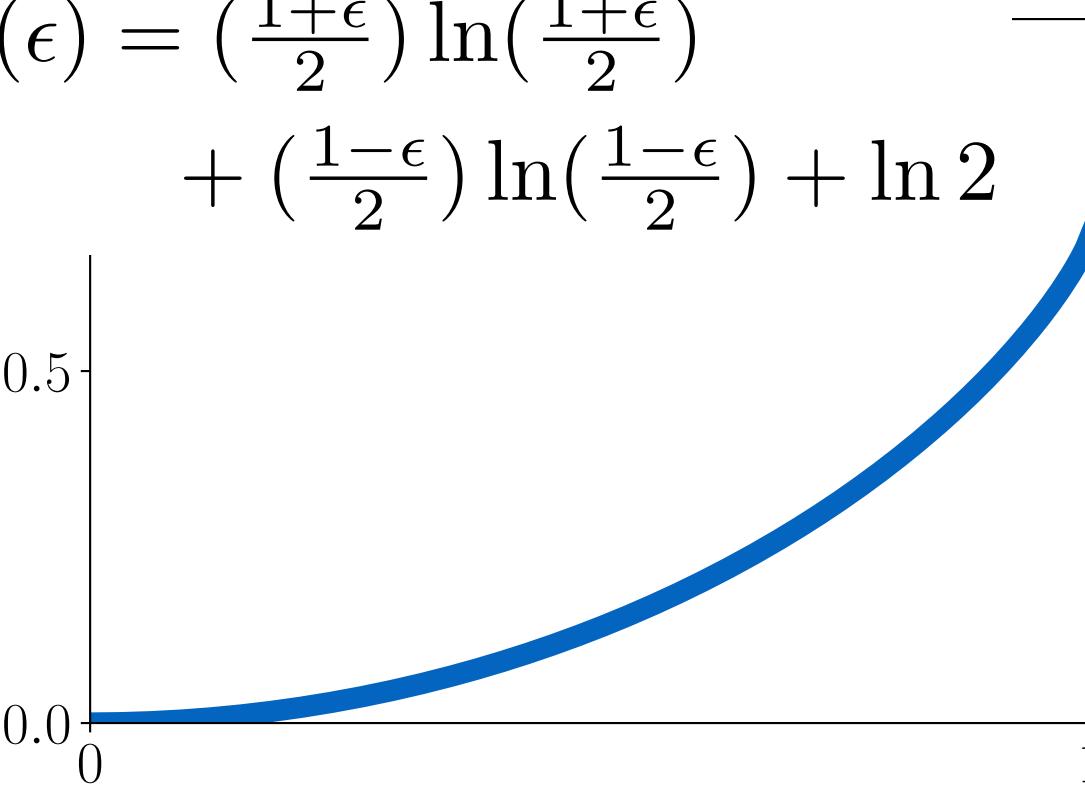
● L2 loss



● Log loss



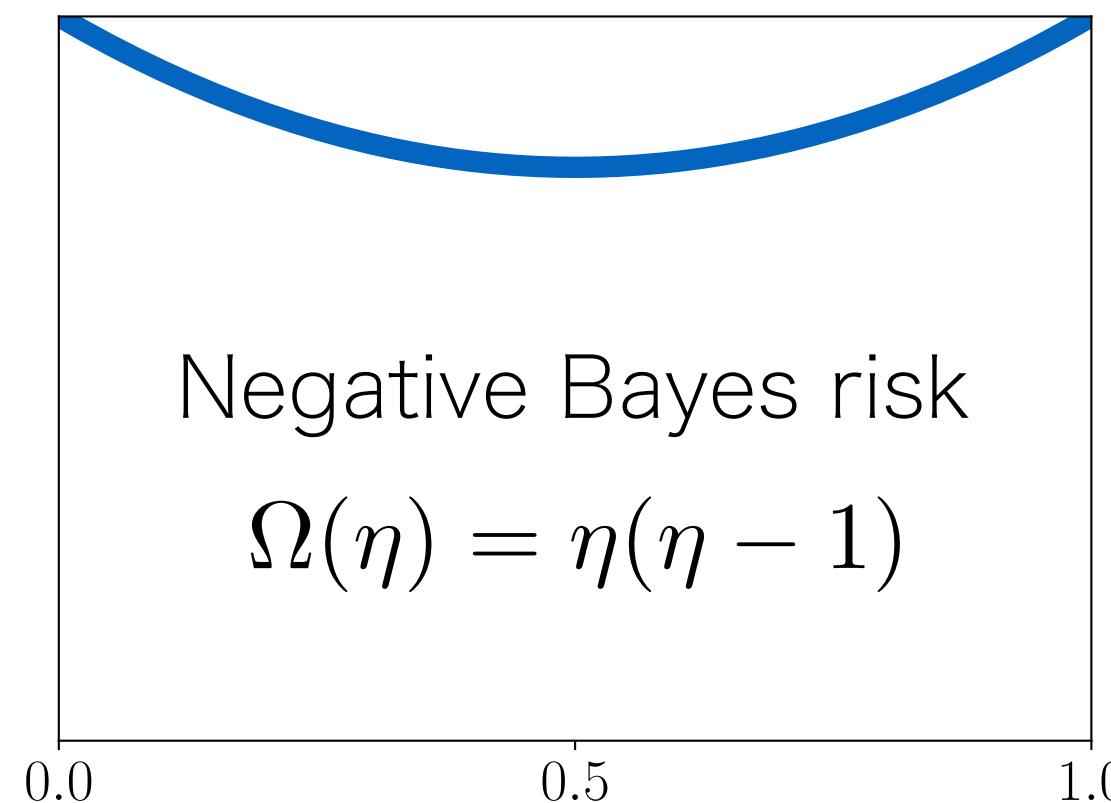
$$\delta(\epsilon) = \left(\frac{1+\epsilon}{2}\right) \ln\left(\frac{1+\epsilon}{2}\right) + \left(\frac{1-\epsilon}{2}\right) \ln\left(\frac{1-\epsilon}{2}\right) + \ln 2$$



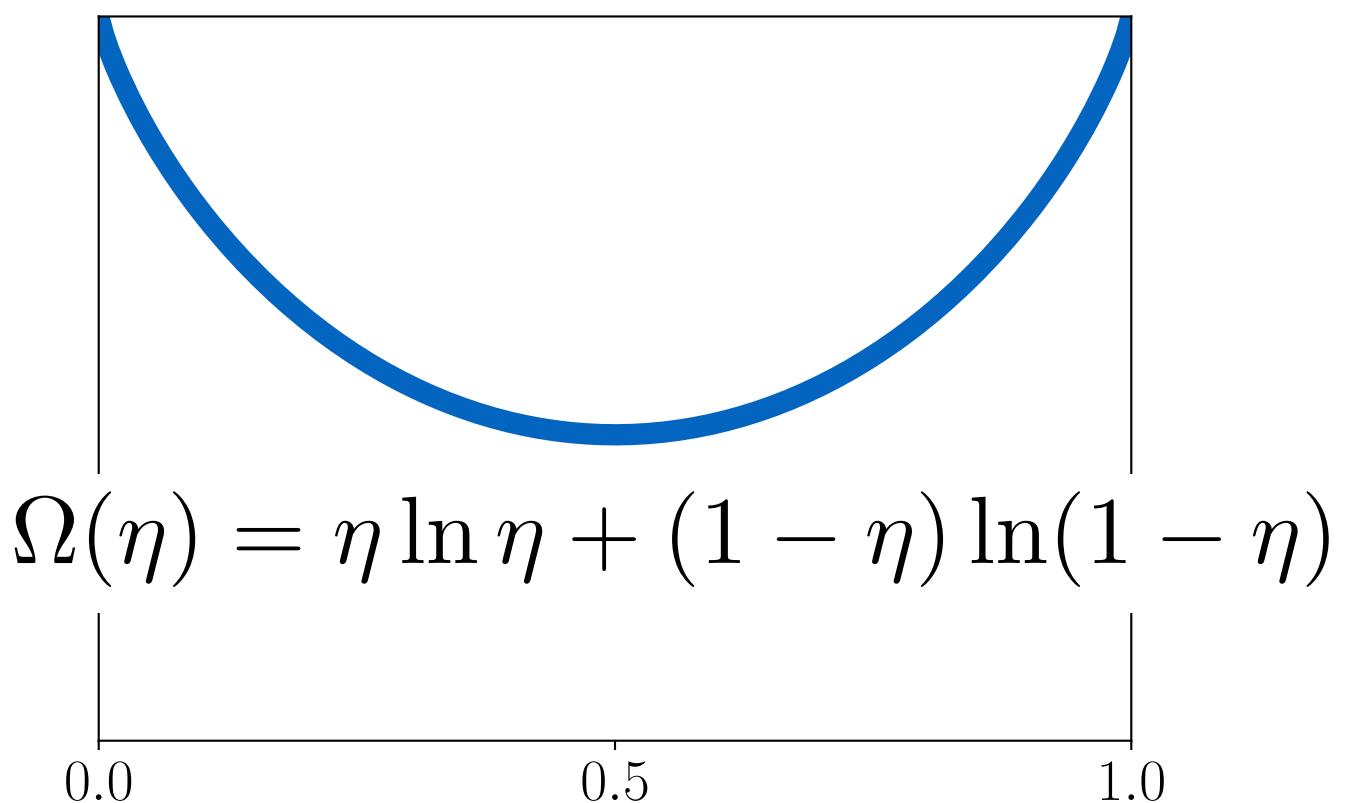
$(\Omega = -\underline{L}_\ell)$

Examples

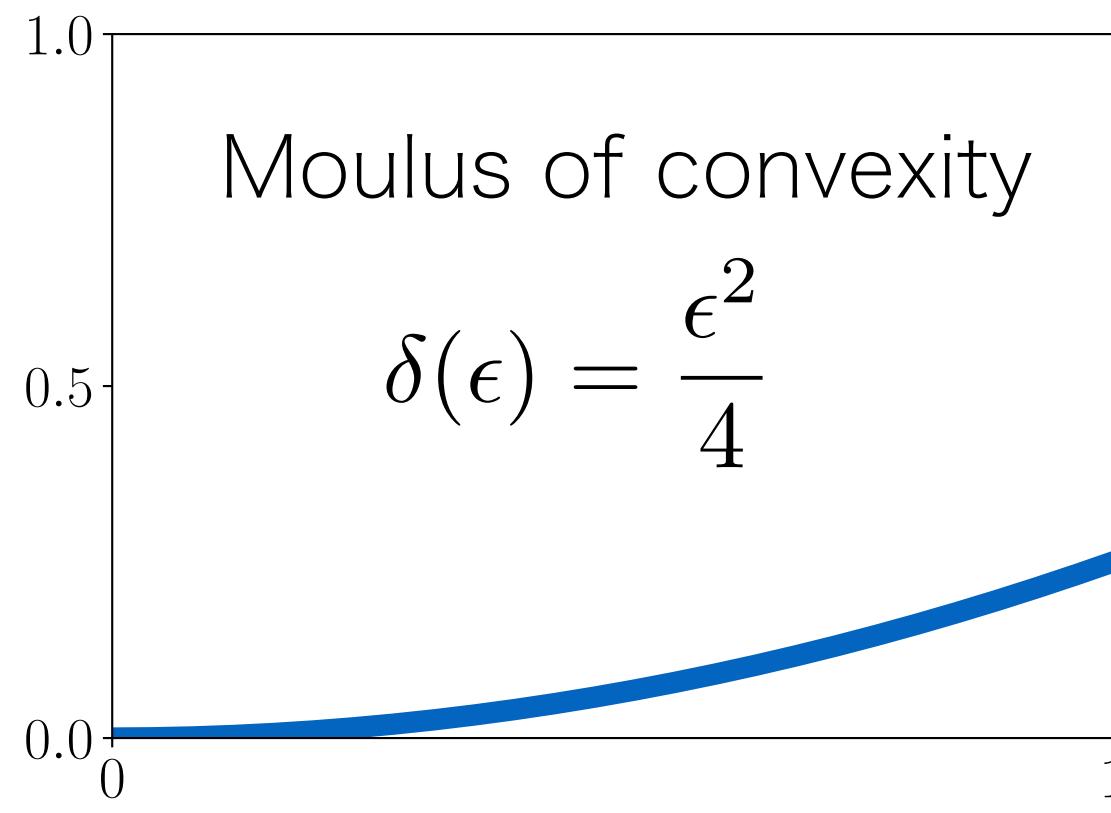
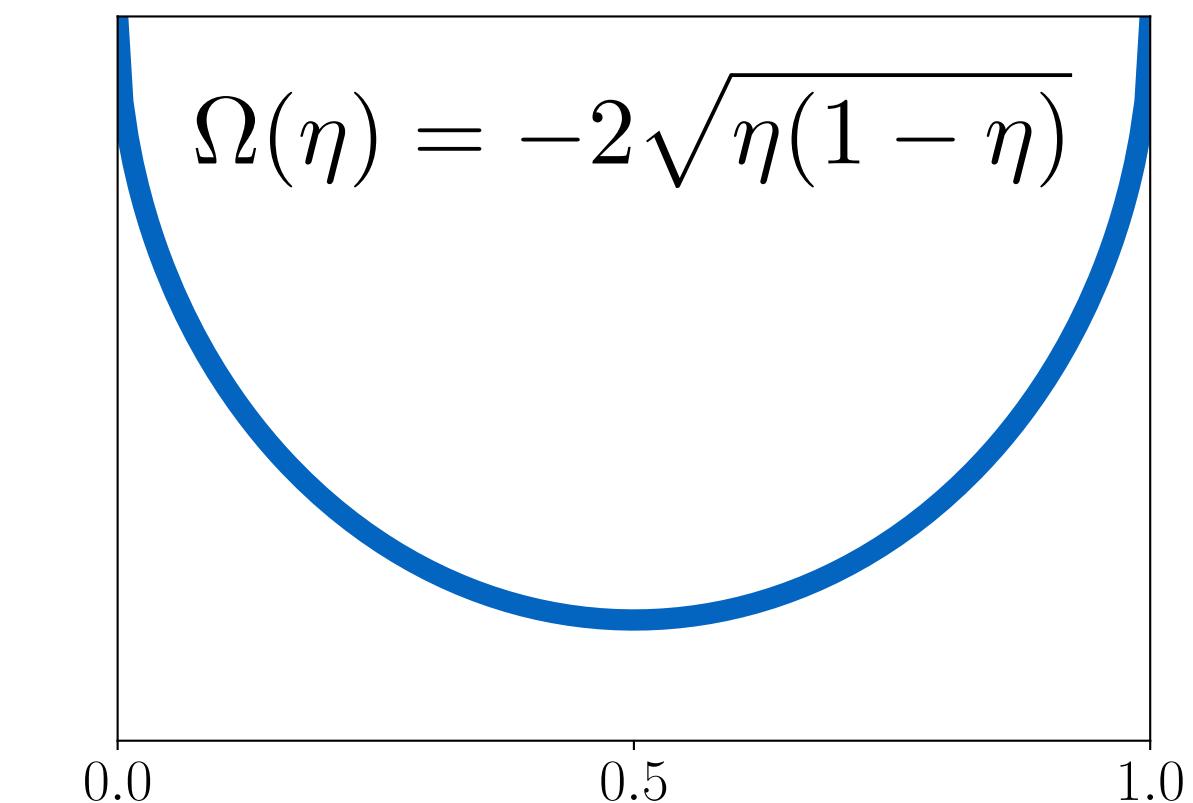
● L2 loss



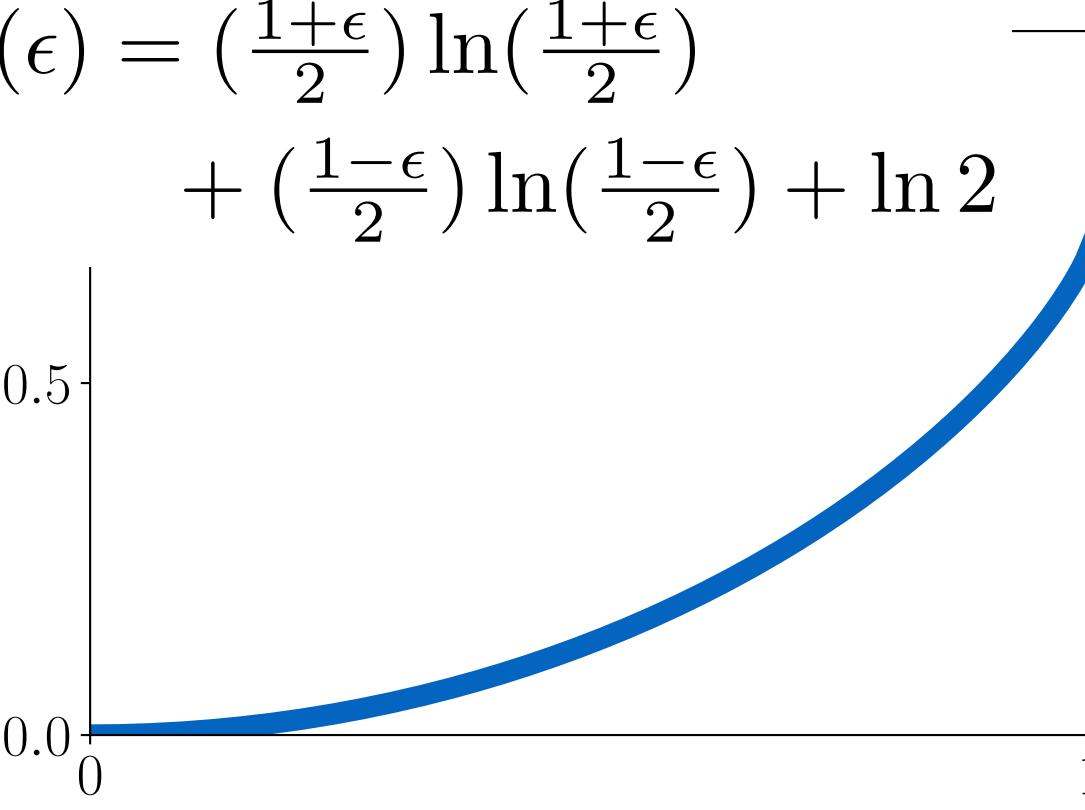
● Log loss



● Exponential (Boosting) loss



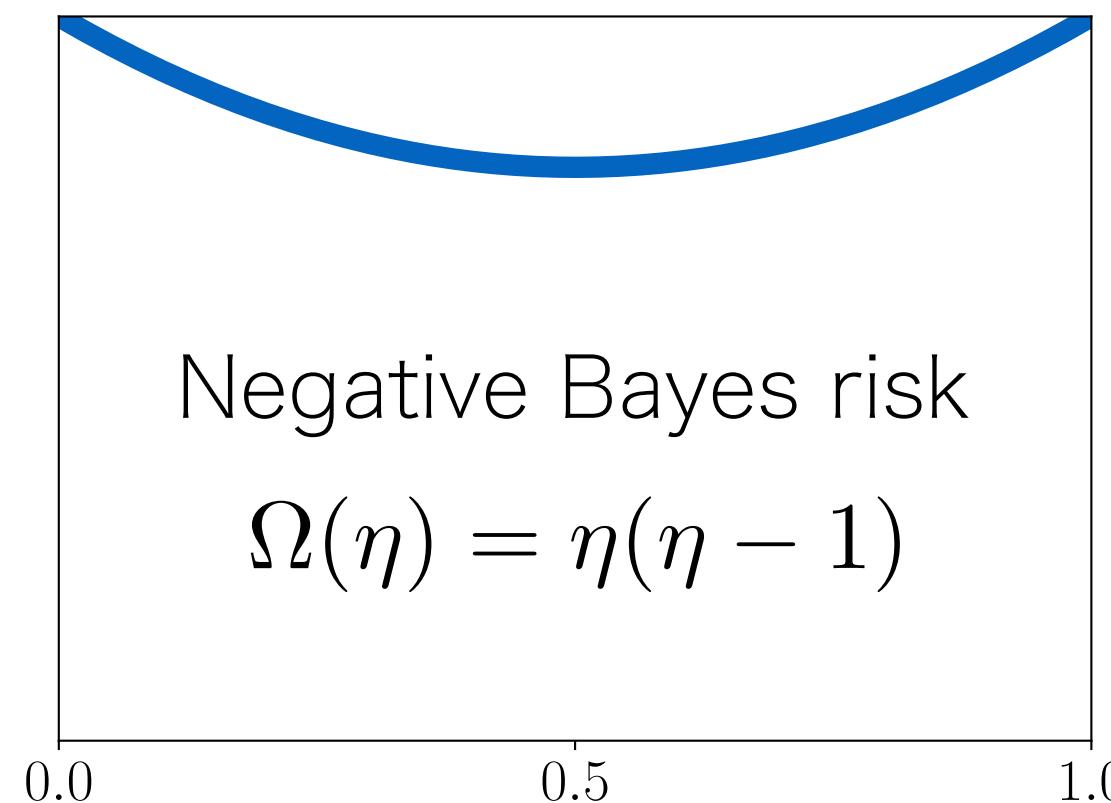
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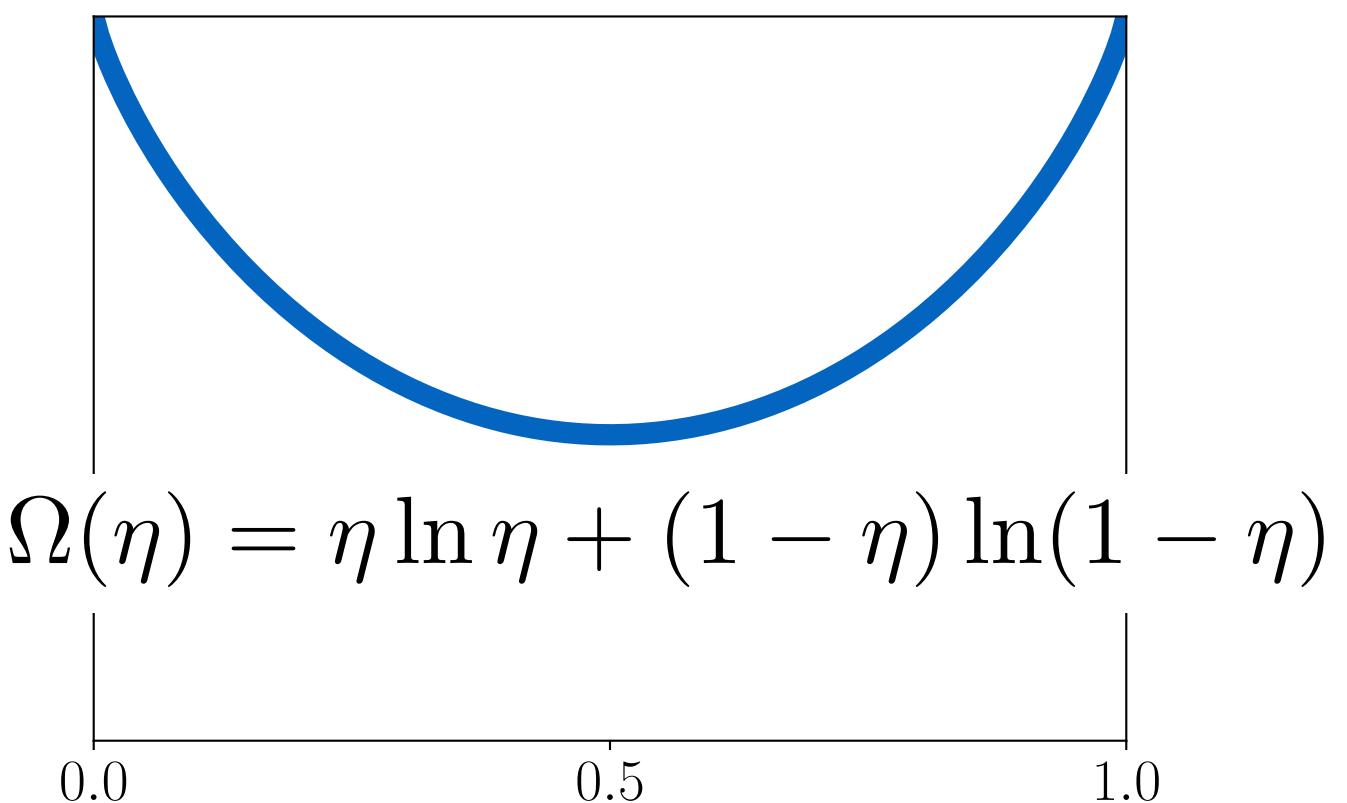
($\Omega = -\underline{L}_\ell$)

Examples

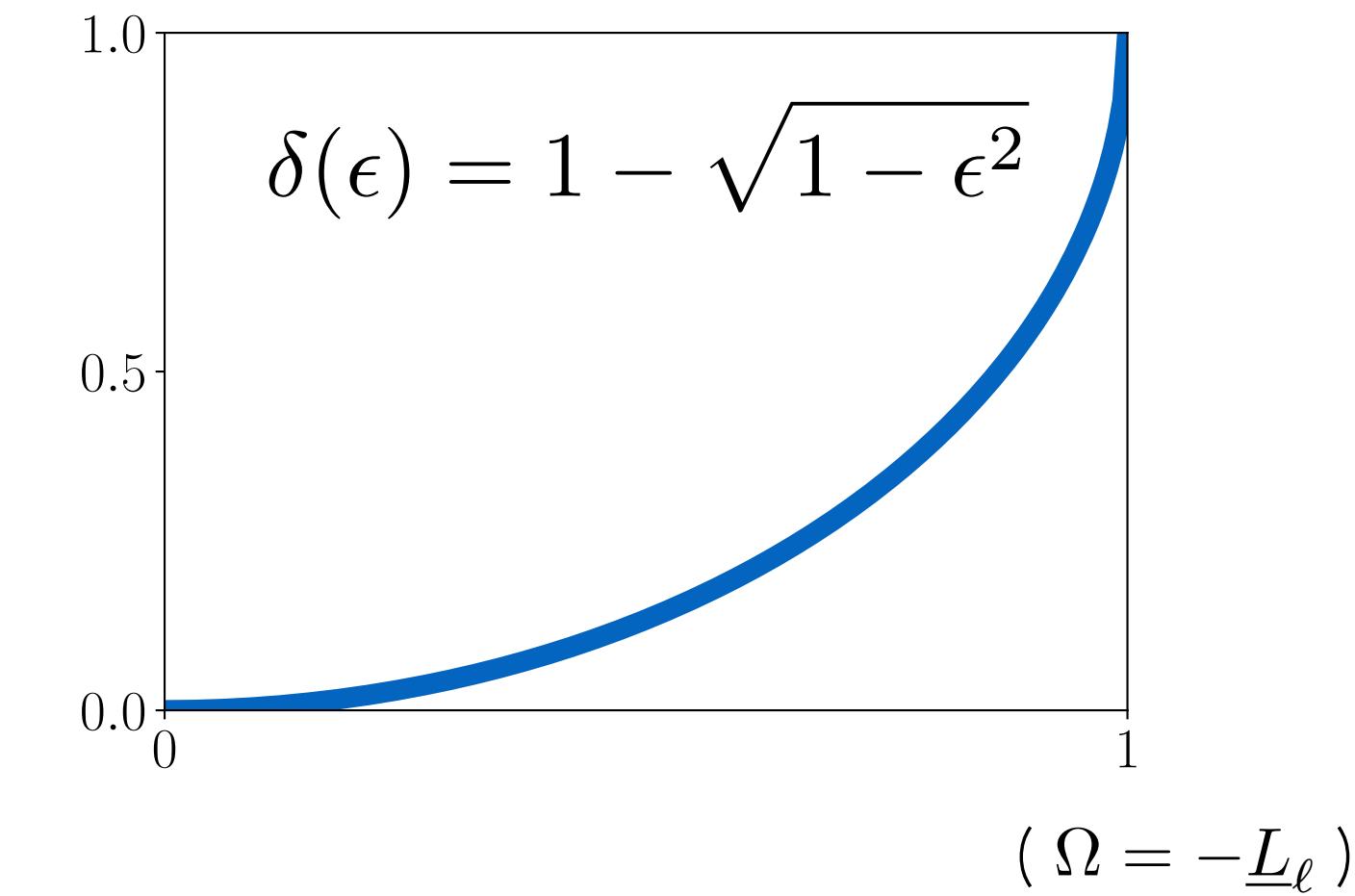
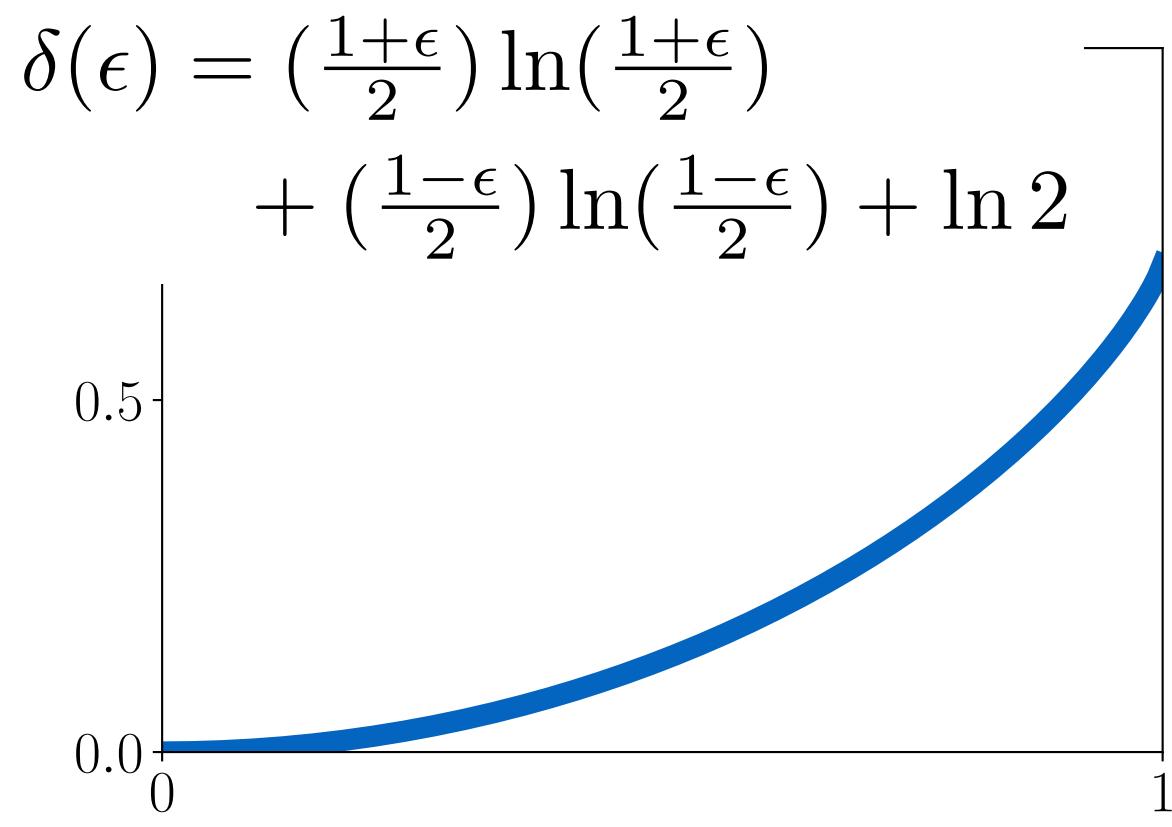
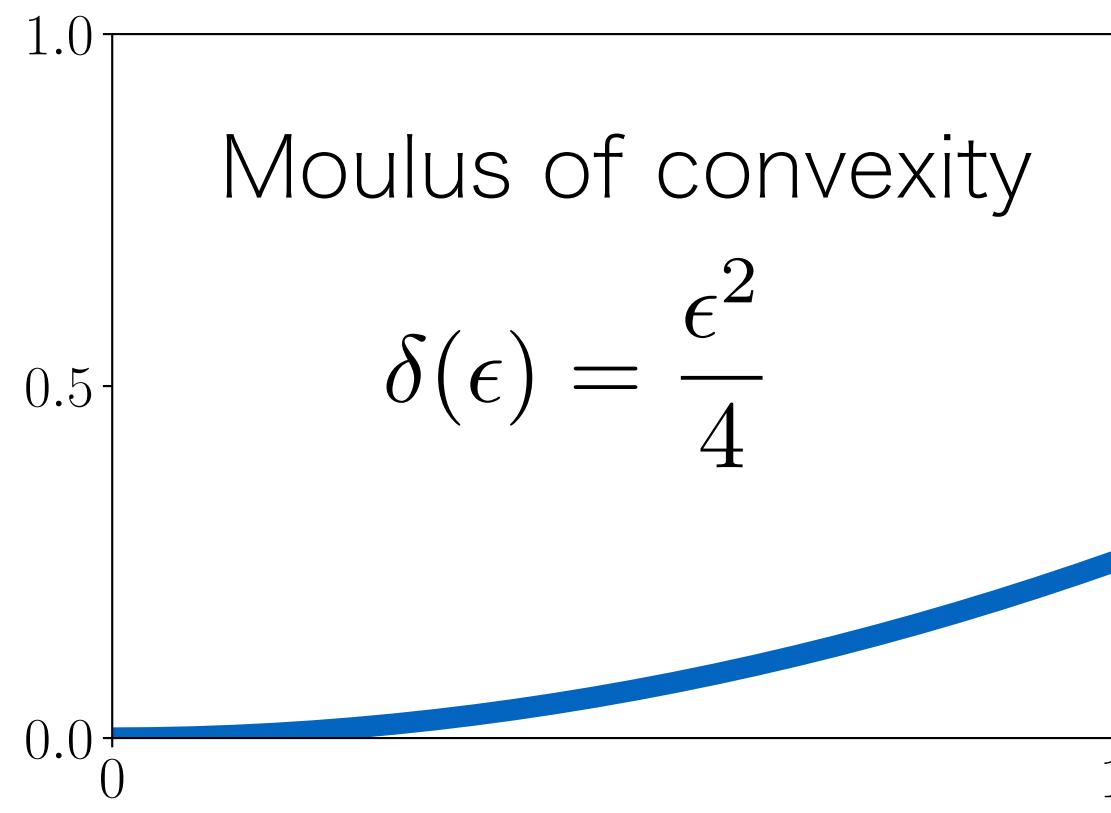
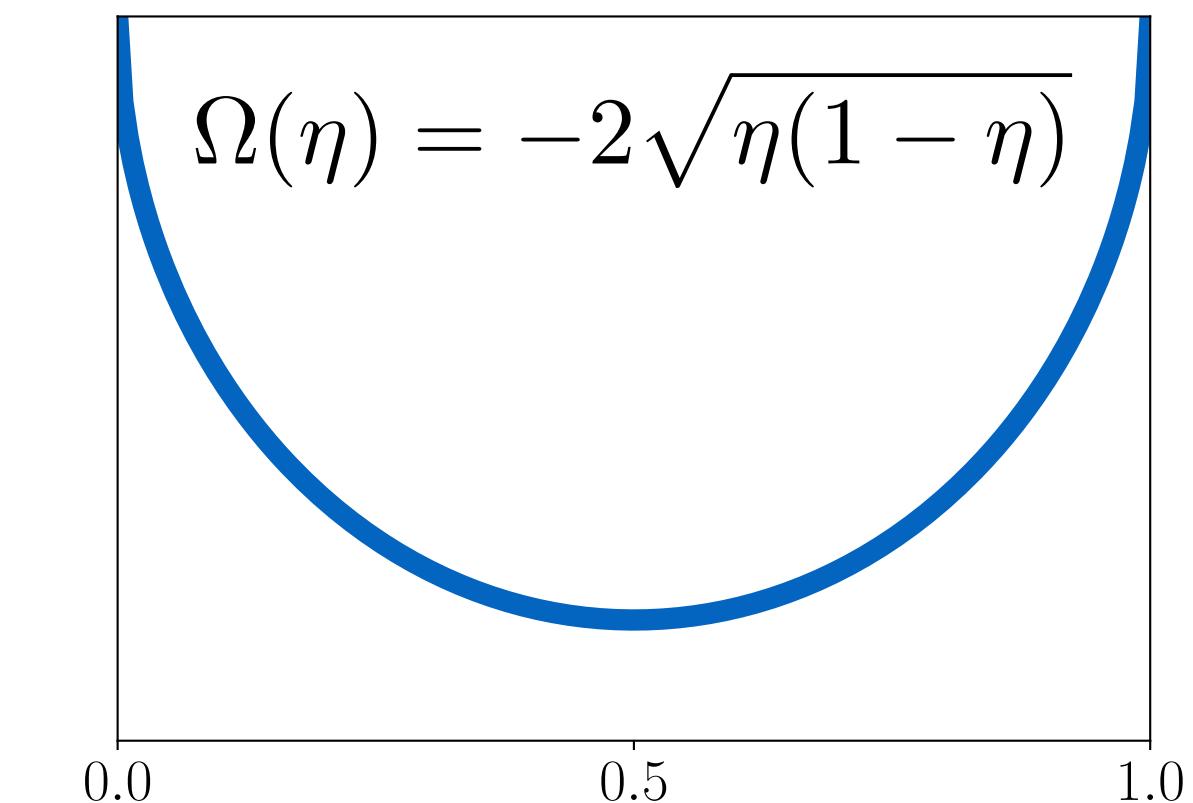
● L2 loss



● Log loss

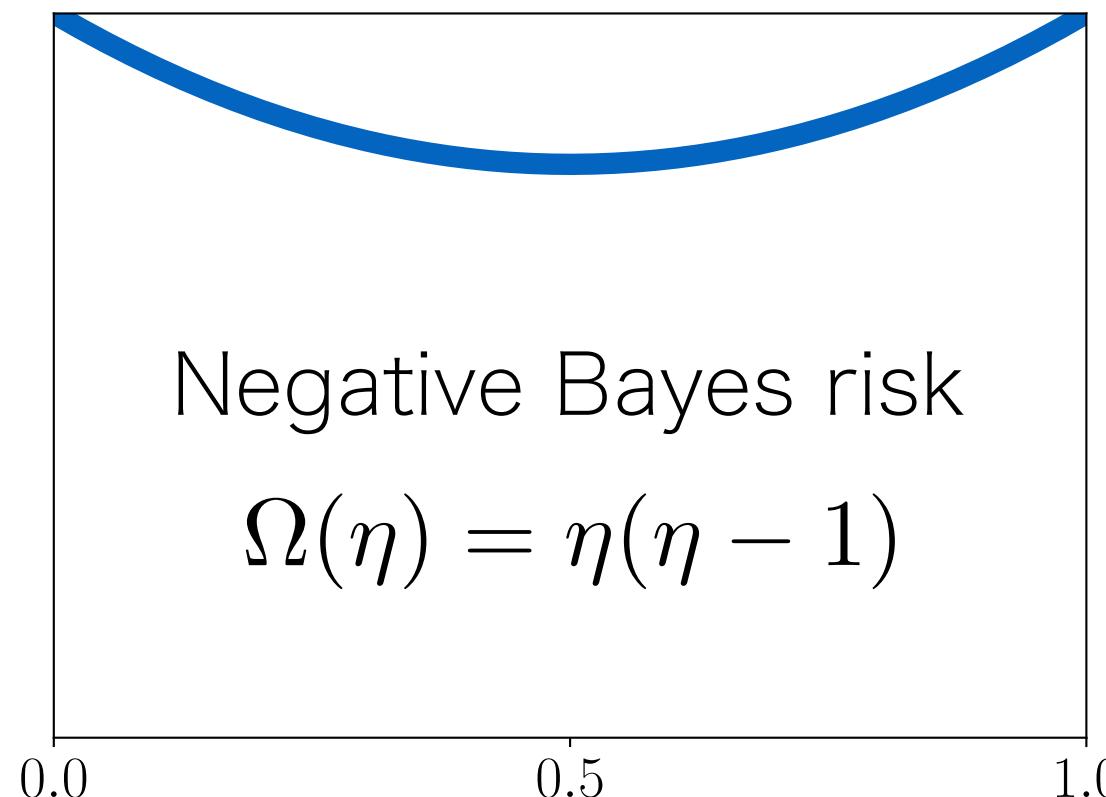


● Exponential (Boosting) loss



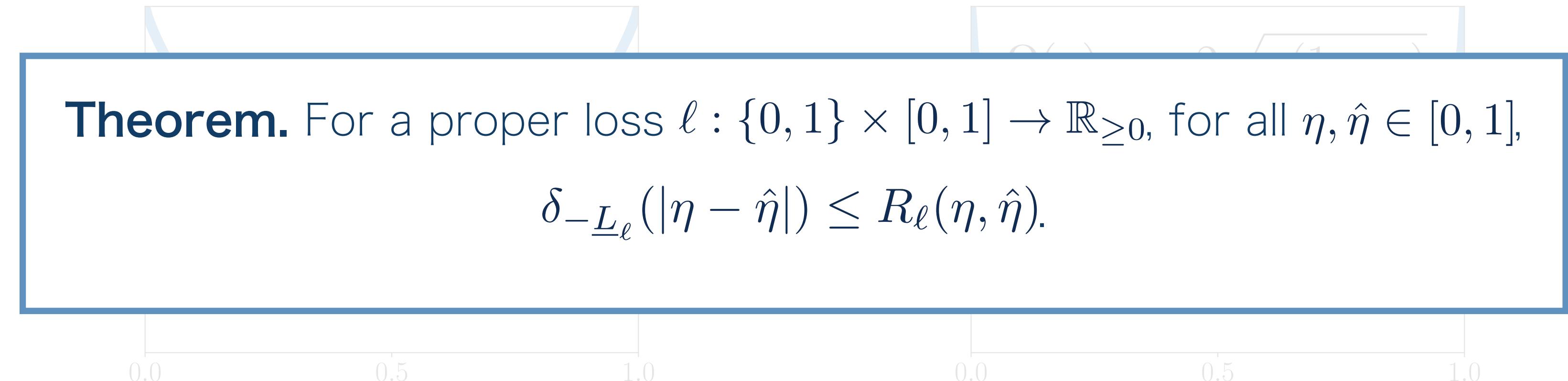
Examples

- L2 loss

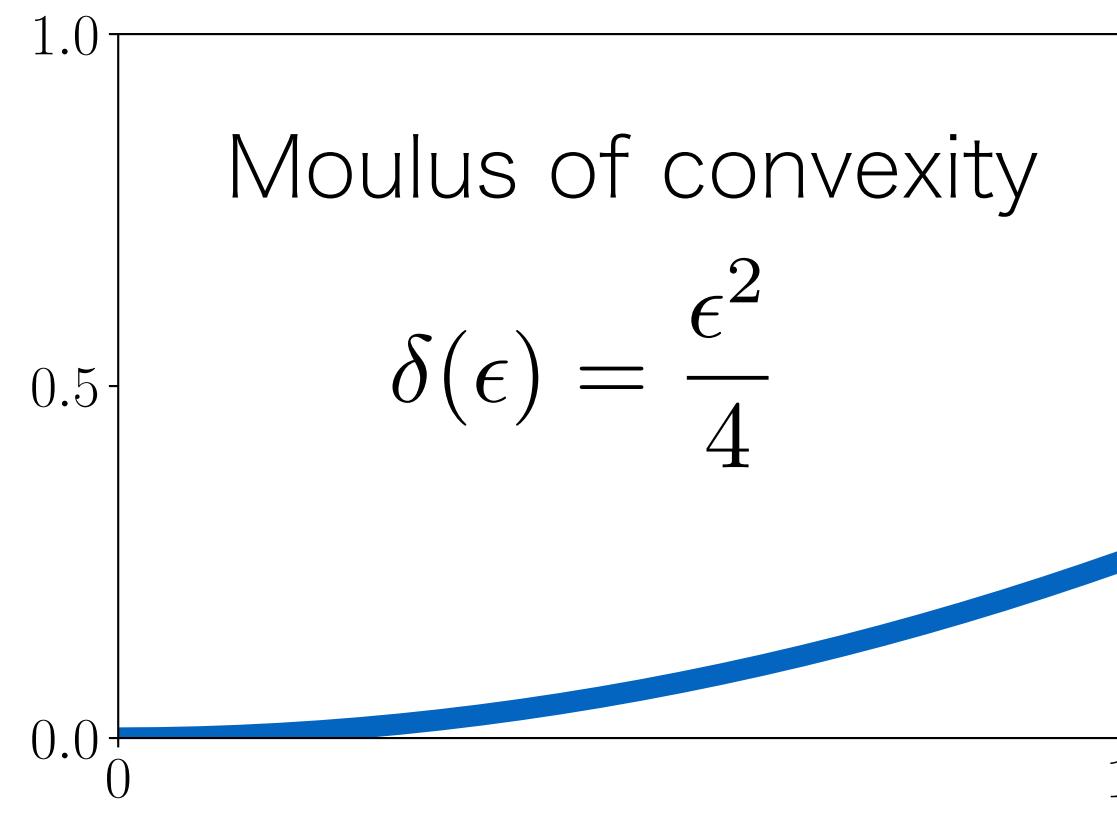


Negative Bayes risk
 $\Omega(\eta) = \eta(\eta - 1)$

- Log loss



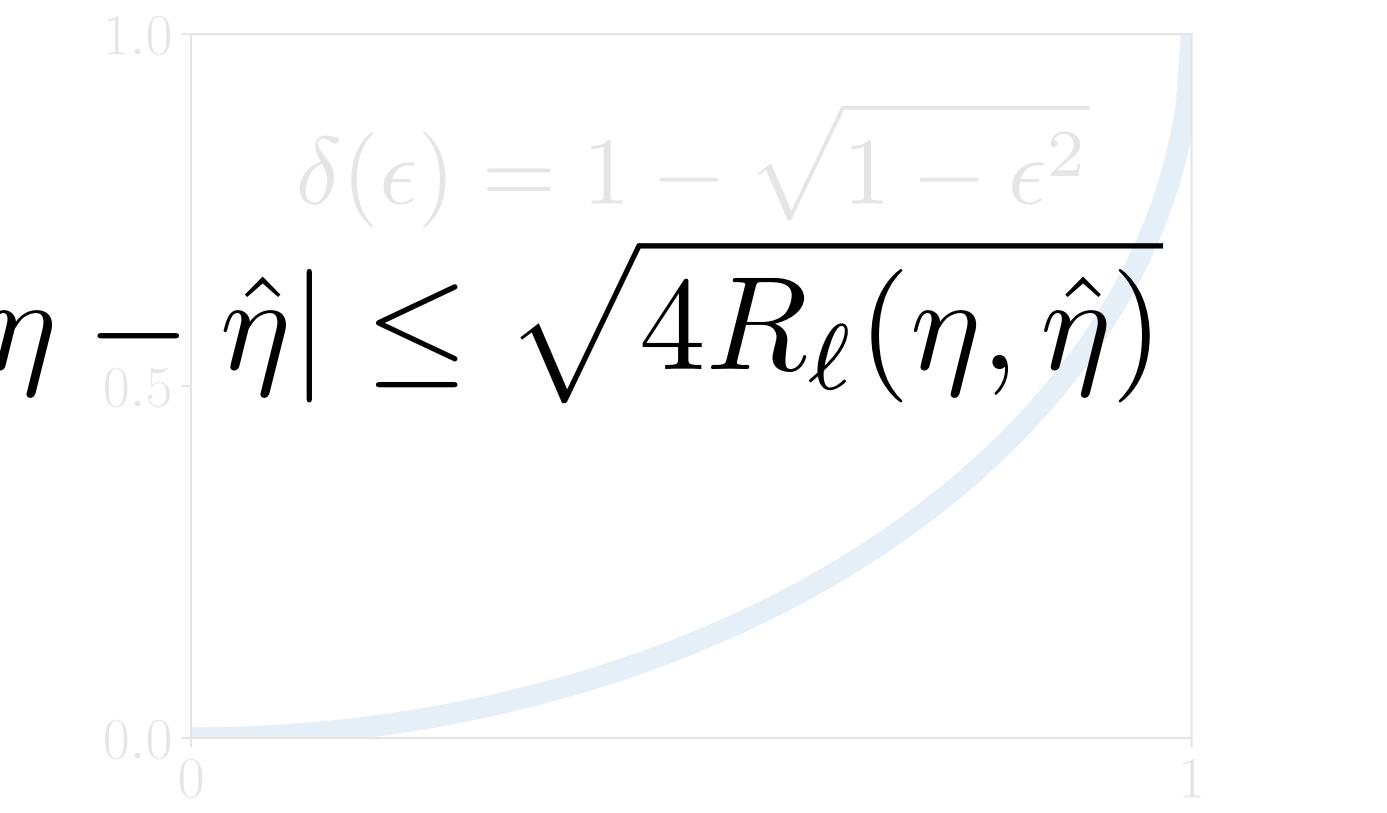
Theorem. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, for all $\eta, \hat{\eta} \in [0, 1]$,

$$\delta_{-\underline{L}_\ell}(|\eta - \hat{\eta}|) \leq R_\ell(\eta, \hat{\eta}).$$


Moulus of convexity
 $\delta(\epsilon) = \frac{\epsilon^2}{4}$

$$\begin{aligned} \delta(\epsilon) &= \left(\frac{1+\epsilon}{2}\right) \ln\left(\frac{1+\epsilon}{2}\right) \\ &\quad + \left(\frac{1-\epsilon}{2}\right) \ln\left(\frac{1-\epsilon}{2}\right) + \ln 2 \\ \frac{1}{4}|\eta - \hat{\eta}|^2 &\leq R_\ell(\eta, \hat{\eta}) \end{aligned}$$

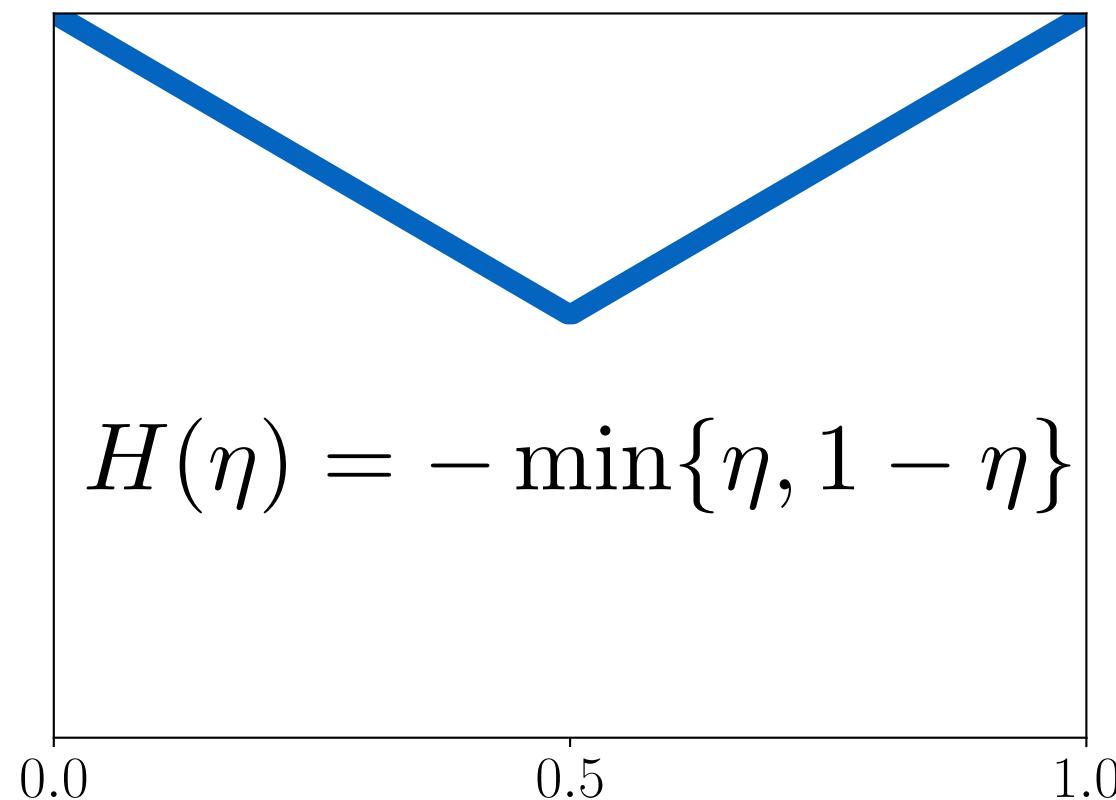
\implies



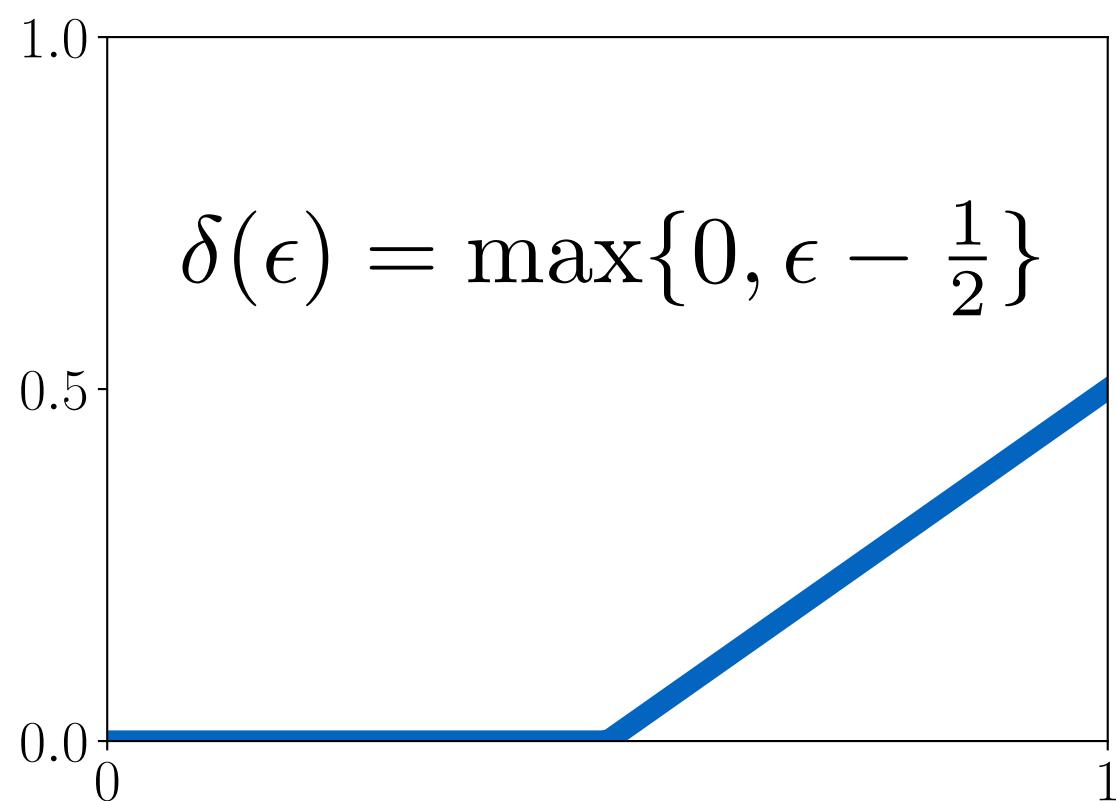
($\Omega = -\underline{L}_\ell$)

Examples

- L1 loss



Theorem. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, for all $\eta, \hat{\eta} \in [0, 1]$,

$$\delta_{-\underline{L}_\ell}(|\eta - \hat{\eta}|) \leq R_\ell(\eta, \hat{\eta}).$$


$$\begin{aligned} \max \left\{ 0, |\eta - \hat{\eta}| - \frac{1}{2} \right\} &\leq R_\ell(\eta, \hat{\eta}) \\ \implies |\eta - \hat{\eta}| &\leq R_\ell(\eta, \hat{\eta}) + \frac{1}{2} \quad (\text{vacuous}) \end{aligned}$$

($\Omega = -\underline{L}_\ell$)

Outline

● **Q.** How should we assess probability estimates?

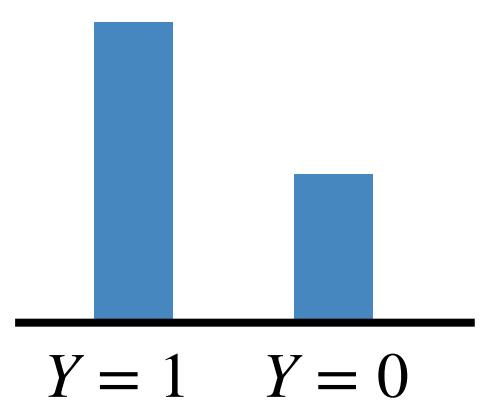
- ❖ Proper losses

● **Q.** How can estimated probabilities be used for other tasks?

- ❖ Regret bounds

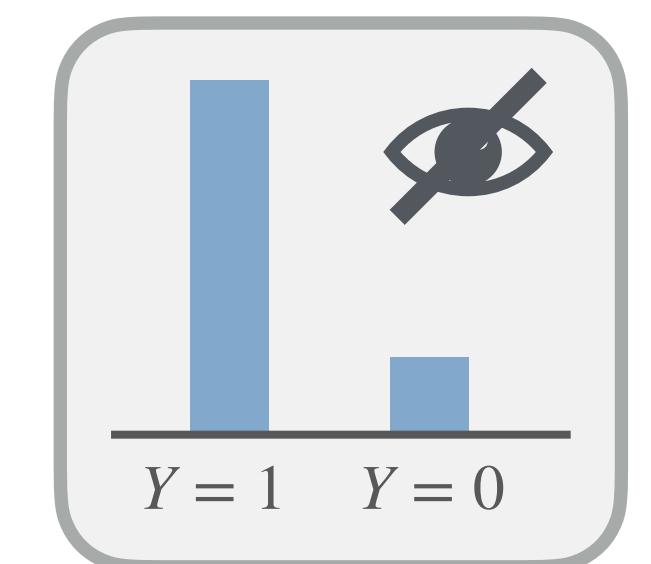
● **Q.** How to compare different loss functions?

- ❖ Order function of moduli



Estimate $\hat{\eta}$

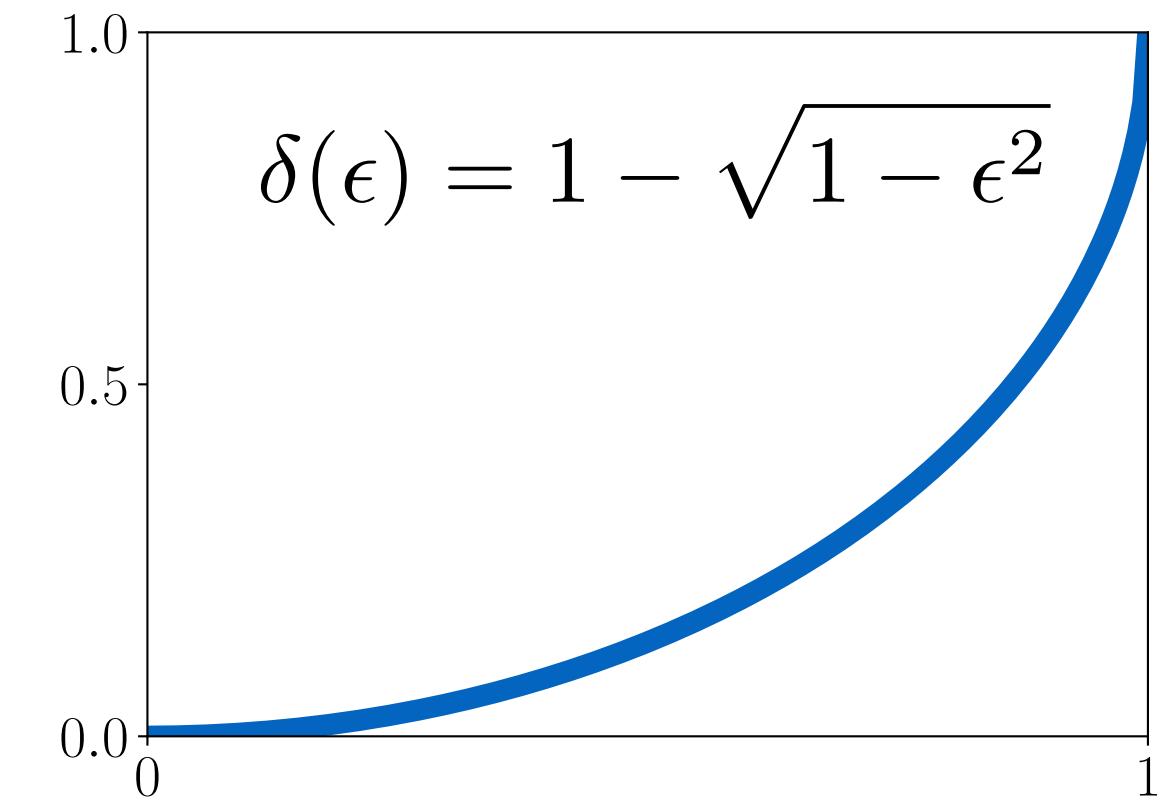
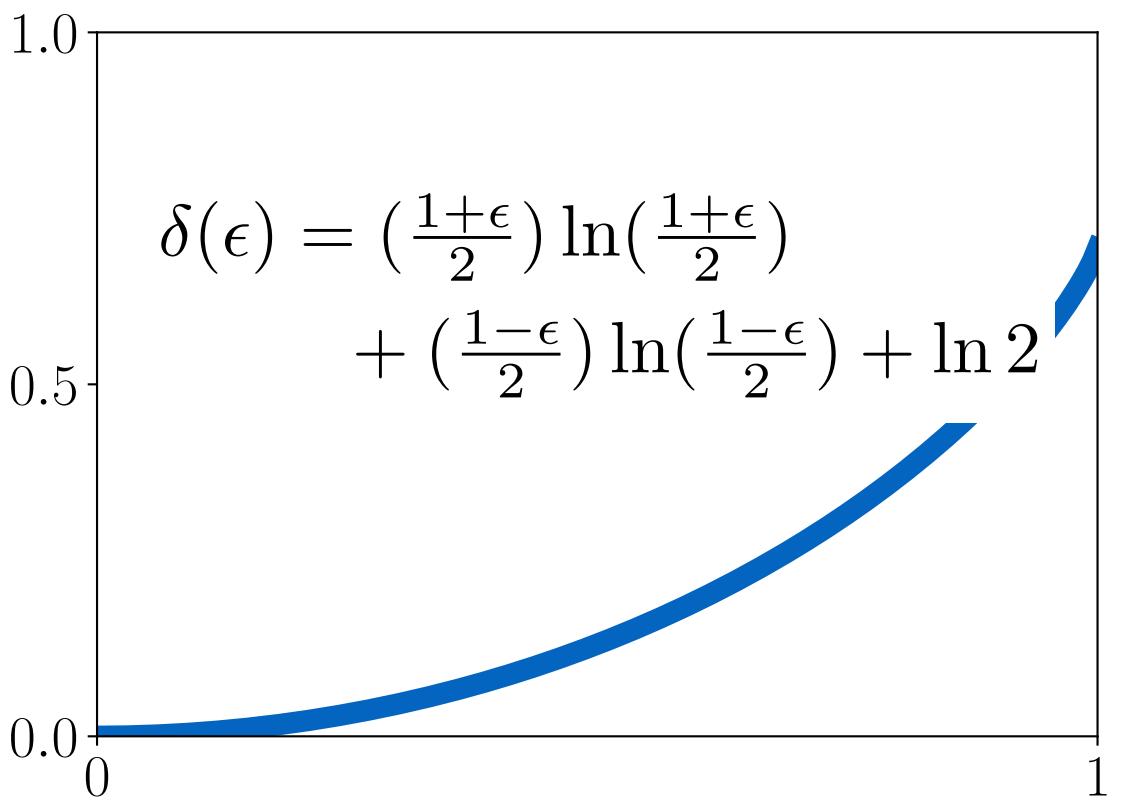
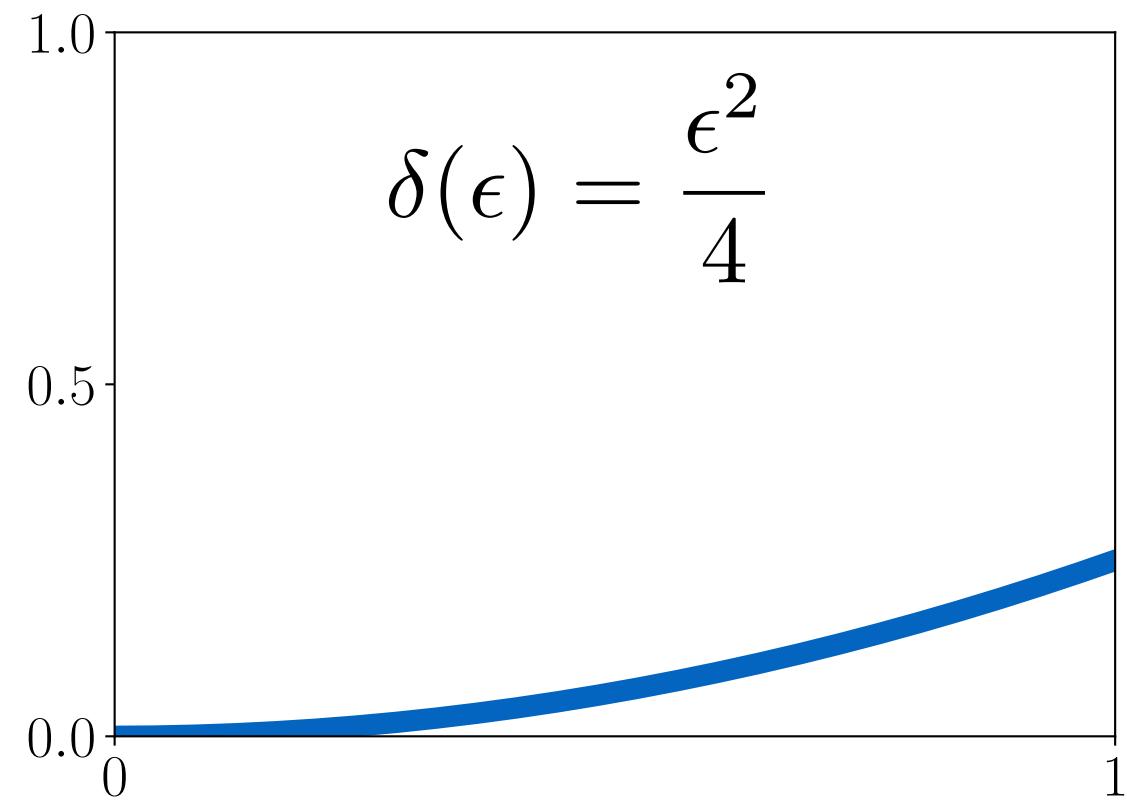
$$\text{dist}(\eta, \hat{\eta})$$



True η

Can we obtain more meaningful bounds?

- L1 regret bounds are characterized by moduli



❖ Moduli are not friendly for us

- Q. Can we evaluate moduli by polynomials?

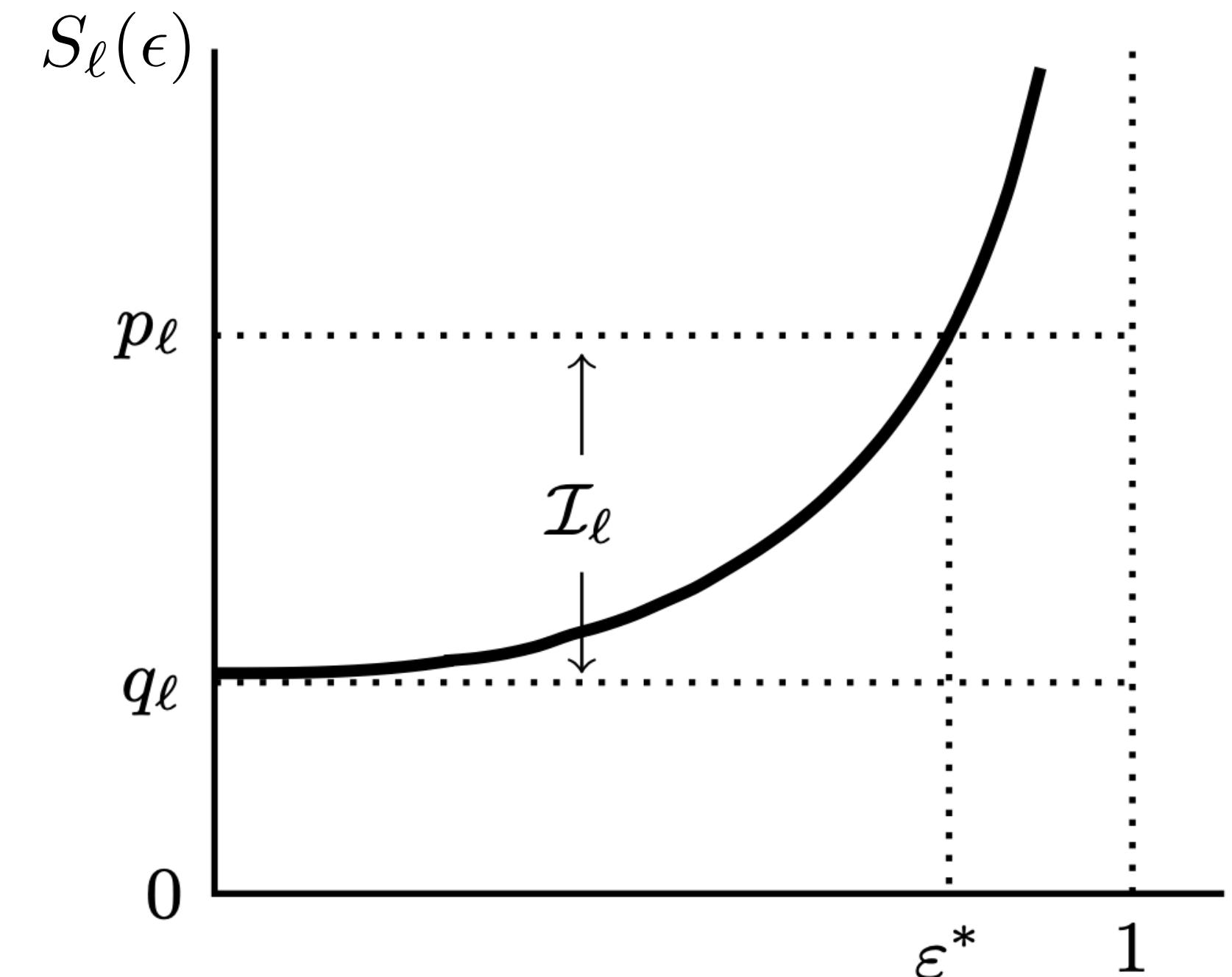
❖ For some r, R , $\epsilon^r \leq \delta(\epsilon) \leq \epsilon^R$

Polynomial bounds of moduli

Definition [Simonenko 1964]. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, order function $S_\ell : (0, 1] \rightarrow \overline{\mathbb{R}}$ is

$$S_\ell(t) := \frac{t(\delta_{-\underline{L}_\ell}^{**})'(t)}{\delta_{-\underline{L}_\ell}^{**}(t)}.$$

- Order function tells how many orders polynomial approximation of $\delta_{-\underline{L}_\ell}^{**}$ is at a given point t
 - ❖ Take a point ϵ^*
 - ❖ Take sup and inf in $[0, \epsilon^*]$ to define p_ℓ and q_ℓ
 - ❖ p_ℓ and q_ℓ provides us polynomial bounds and their orders (see next page)



Example for log loss

Polynomial bounds of moduli

Definition [Simonenko 1964]. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, order function $S_\ell : (0, 1] \rightarrow \overline{\mathbb{R}}$ is

$$S_\ell(t) := \frac{t(\delta_{-\underline{L}_\ell}^{**})'(t)}{\delta_{-\underline{L}_\ell}^{**}(t)}.$$

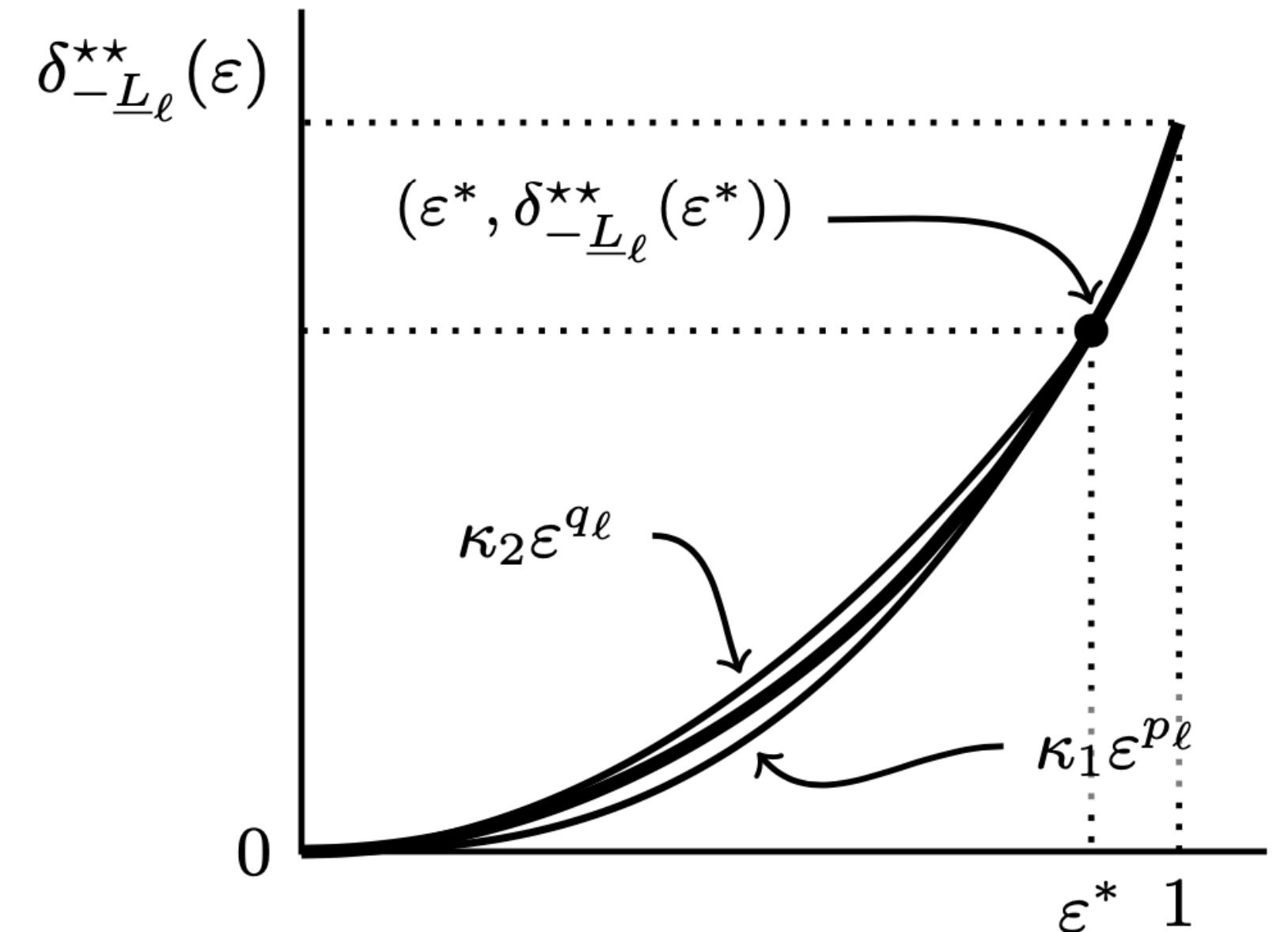
Theorem. For a strictly proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$,

$\epsilon_* \in (0, 1]$, define $p_\ell := \sup_{t \in (0, \epsilon_*]} S_\ell(t)$ and $q_\ell := \inf_{t \in (0, \epsilon_*]} S_\ell(t)$.

Then, for all $\epsilon \in [0, \epsilon_*]$, we have

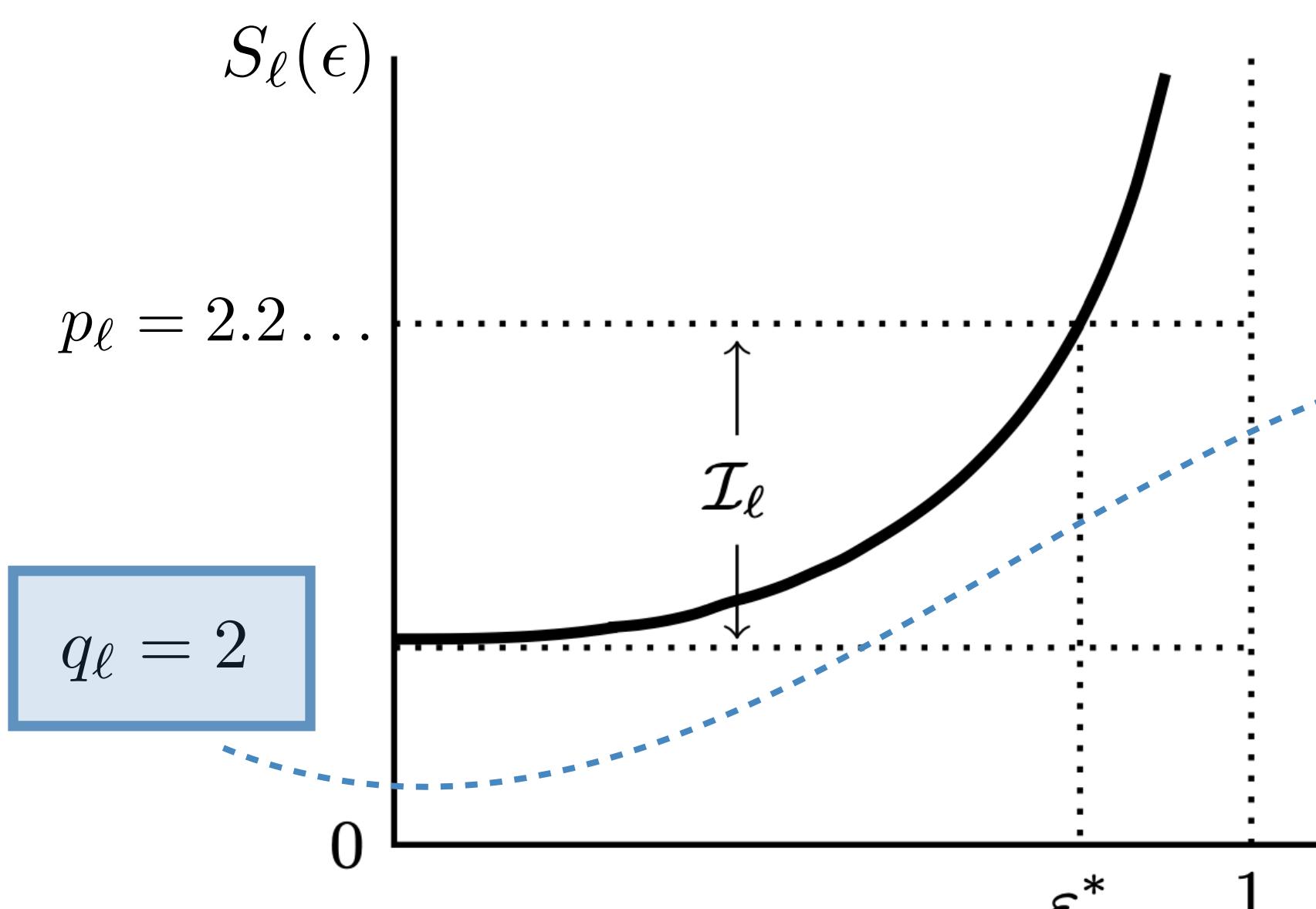
$$\kappa_1 \epsilon^{p_\ell} \leq \delta_{-\underline{L}_\ell}^{**}(\epsilon) \leq \kappa_2 \epsilon^{q_\ell},$$

where $\kappa_1 := \frac{\delta_{-\underline{L}_\ell}^{**}(\epsilon_*)}{\epsilon_*^{p_\ell}}$ and $\kappa_2 := \frac{\delta_{-\underline{L}_\ell}^{**}(\epsilon_*)}{\epsilon_*^{q_\ell}}$.

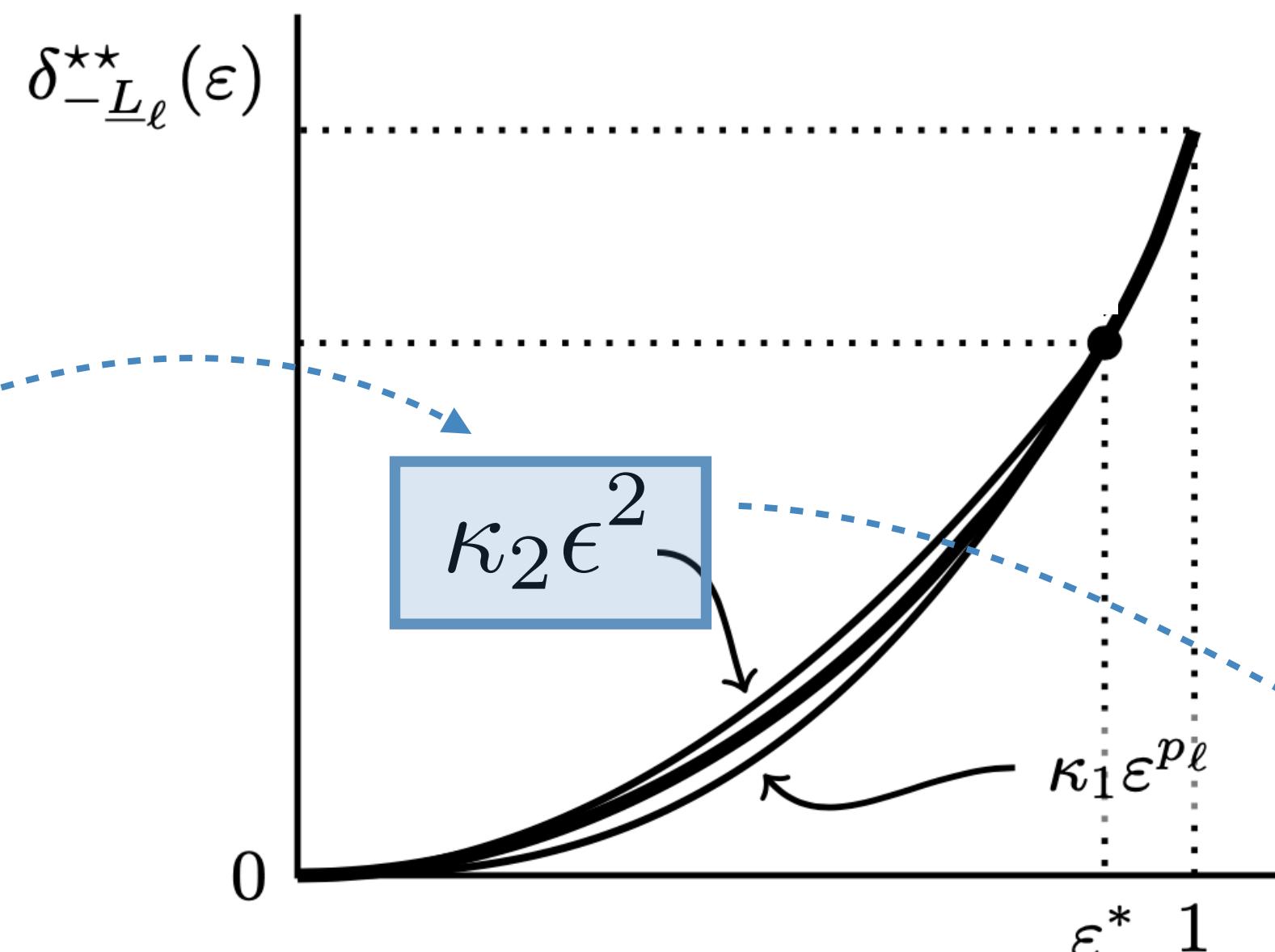


Examples

- Log loss $\delta(\epsilon) = \left(\frac{1+\epsilon}{2}\right) \ln\left(\frac{1+\epsilon}{2}\right) + \left(\frac{1-\epsilon}{2}\right) \ln\left(\frac{1-\epsilon}{2}\right) + \ln 2$



Order function



$$\begin{aligned} \text{Modulus } \delta(\epsilon) &= O(\epsilon^2) \\ \delta(\epsilon) &= \Omega(\epsilon^{2.2\ldots}) \end{aligned}$$

$$|\eta - \hat{\eta}| \leq R_\ell(\eta, \hat{\eta})^{\frac{1}{2.2\ldots}}$$

Upper bound cannot be better than $R_\ell(\eta, \hat{\eta})^2$

Examples

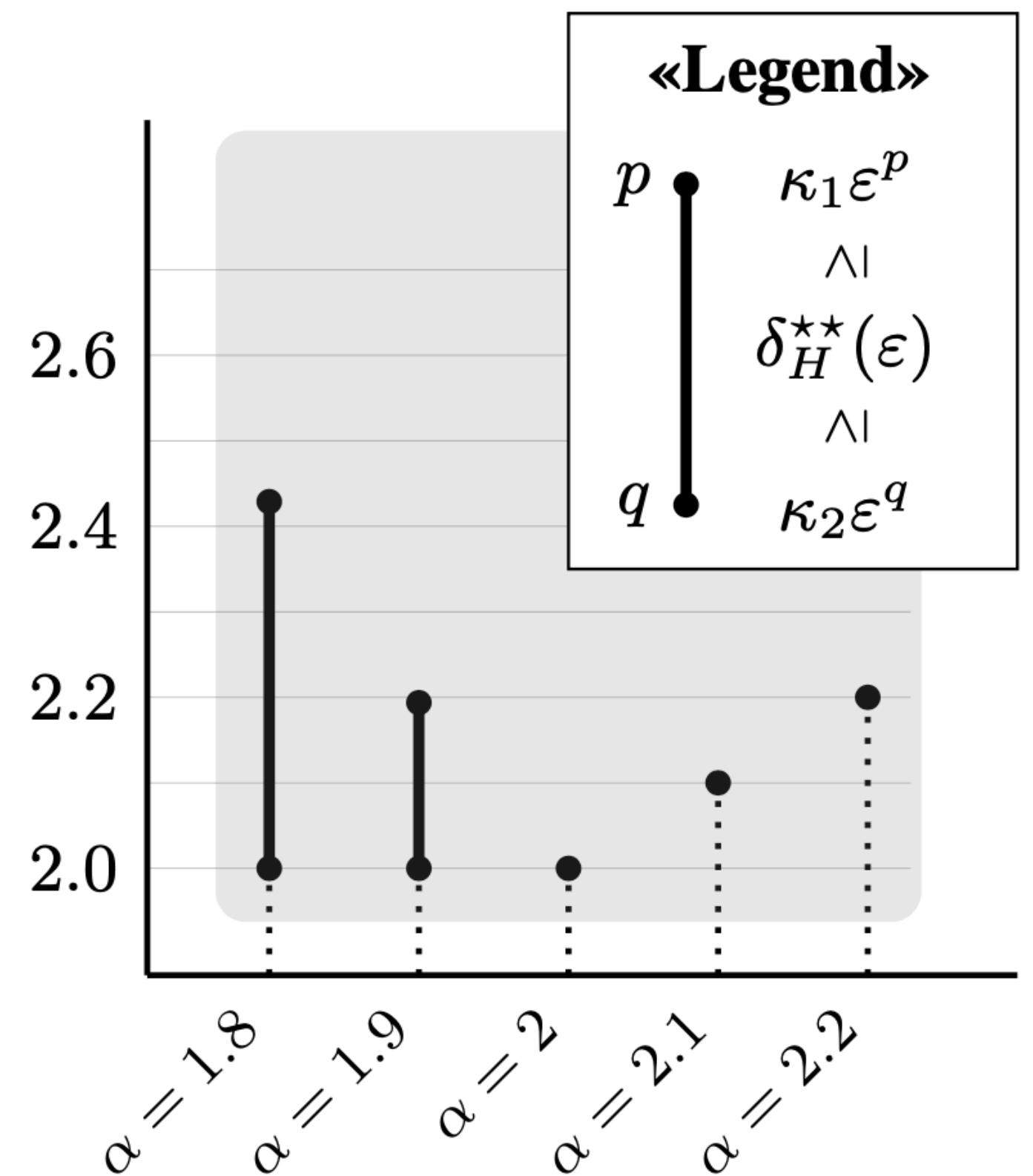
- Polynomial entropies $\Omega(\eta) = |\eta - \frac{1}{2}|^\alpha - \frac{1}{2^\alpha}$
- It reduces to (the associated Bayes risk of) L2 loss when $\alpha = 2$

● Implications

- ❖ No matter how we modulate α , the smallest q_ℓ is 2
- ❖ The upper order p_ℓ is tight when $\alpha = 2$
and we obtain $|\eta - \hat{\eta}| \leq R_\ell(\eta, \hat{\eta})^2$

Reminder

- [↔] For a concave $H : [0, 1] \rightarrow \mathbb{R}$, loss $\ell(y, \hat{\eta}) = H(\hat{\eta}) + (y - \hat{\eta})H'(\hat{\eta})$ is proper
- ❖ Remark: one-to-one correspondence between proper loss and concave function



Summary

- **Proper loss:** a reasonable loss for probabilistic estimation

Definition. $\ell(y, \hat{\eta})$ is strictly proper iff $L_\ell(\eta, \hat{\eta}) = \underline{L}_\ell(\eta) \iff \hat{\eta} = \eta$ for all $\eta \in [0, 1]$.

$$L_\ell(\eta, \hat{\eta}) = \eta\ell(1, \hat{\eta}) + (1 - \eta)\ell(0, \hat{\eta}) \quad \underline{L}_\ell(\eta) = \inf_{\hat{\eta} \in [0, 1]} L_\ell(\eta, \hat{\eta})$$

- **L1 regret bound** is characterized by **modulus of convexity**

Theorem. For a proper loss $\ell : \{0, 1\} \times [0, 1] \rightarrow \mathbb{R}_{\geq 0}$, for all $\eta, \hat{\eta} \in [0, 1]$,

$$\delta_{-\underline{L}_\ell}(|\eta - \hat{\eta}|) \leq R_\ell(\eta, \hat{\eta}).$$

- ❖ Useful for unifying regret bounds of many downstream tasks

