Learning Theory Bridges Loss Functions

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- 2nd-year Ph.D. student @ Sugiyama-Honda-Yokoya Lab
- Research Interests:
  robustness and knowledge transfer via loss function

robustness

Calibrated Surrogate Maximization of Linear-fractional Utility in Binary Classification. (AISTATS2020)

Calibrated Surrogate Losses for Adversarially Robust Classification. (COLT2020)

Calibrated surrogate maximization of Dice. (MICCAI2020)

knowledge transfer

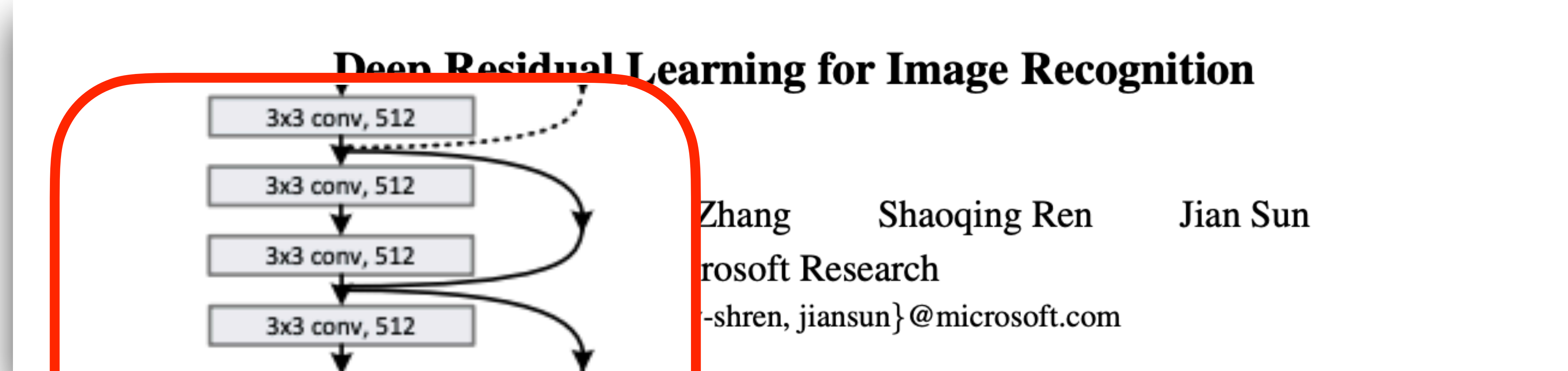
transfer learning

Unsupervised Domain Adaptation Based on Source-guided Discrepancy. (AAAI2019)

similarity learning

Similarity-based Classification: Connecting Similarity Learning to Binary Classification. (preprint)

Classification from Pairwise Similarity and Unlabeled Data. (ICML2018)

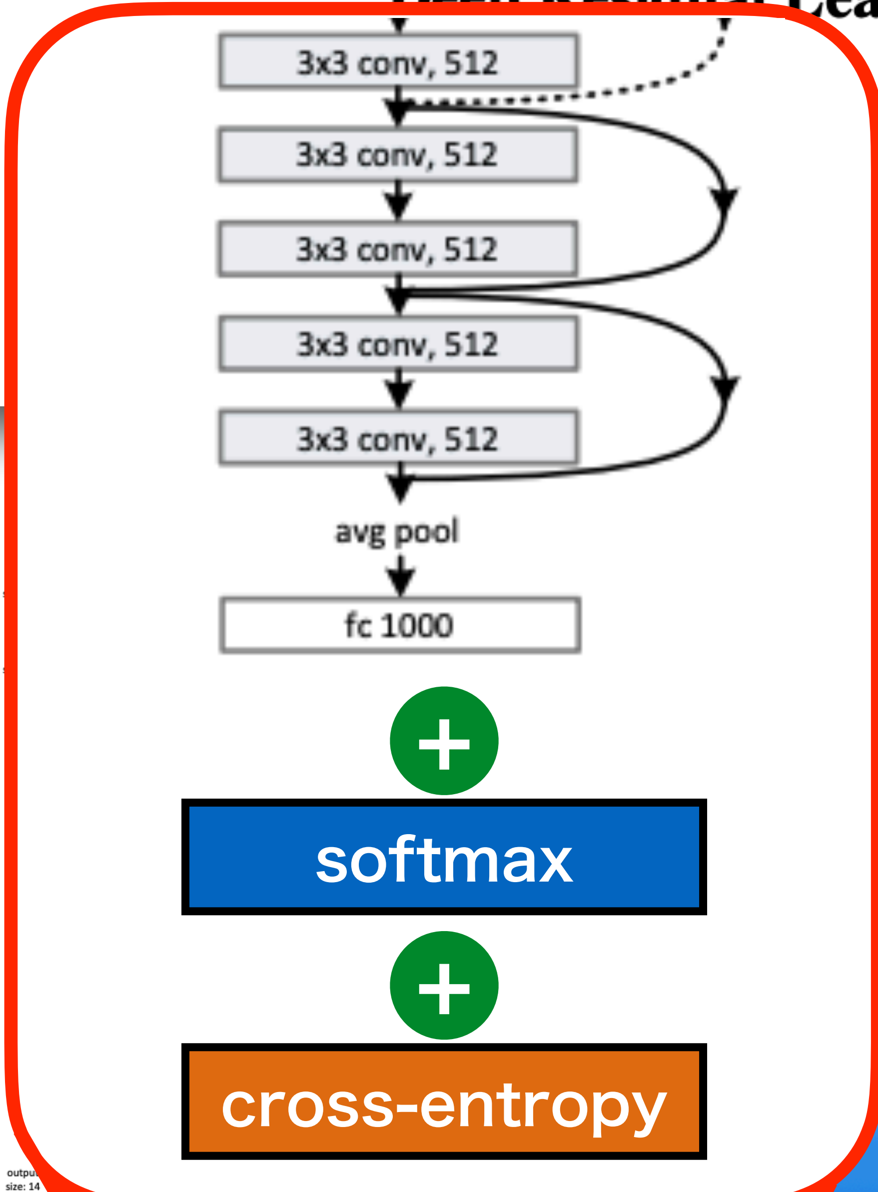


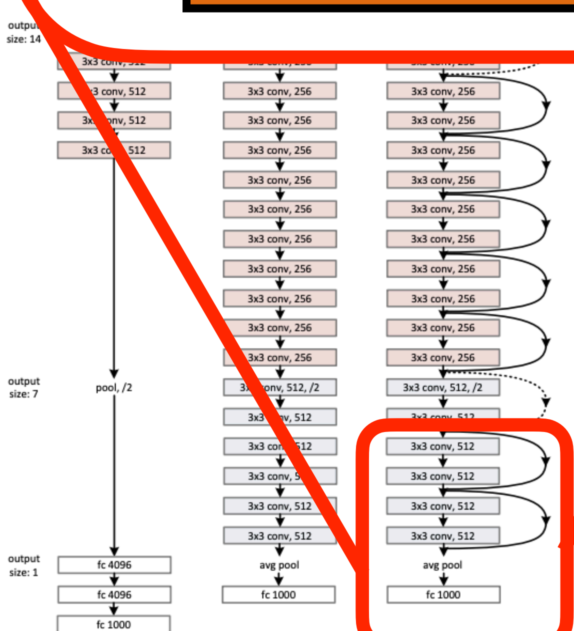
Deep Residual Learning for Image Recognition

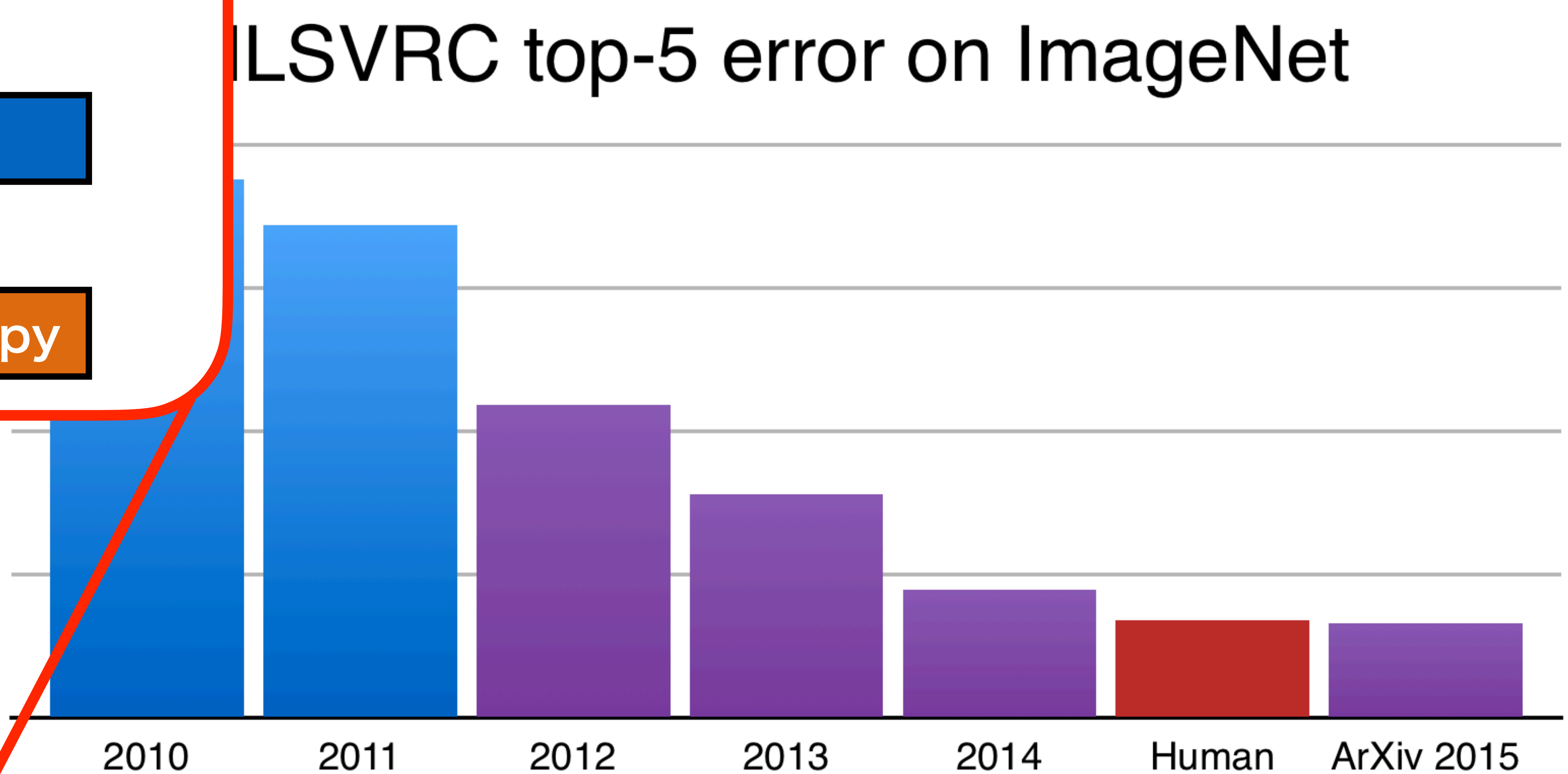
Zhang Shaoqing Ren Jian Sun

rosoft Research

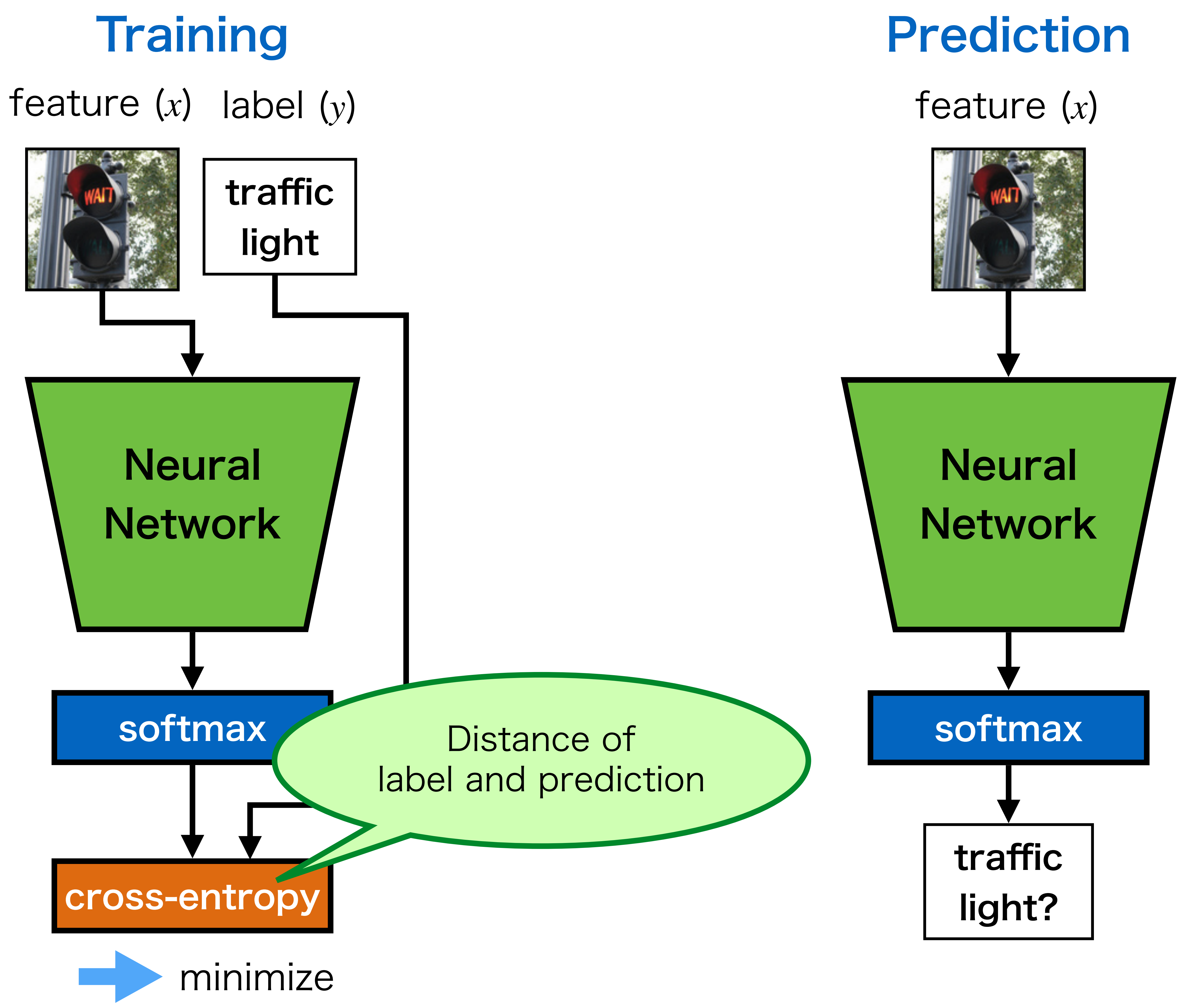
-shren, jiansun}@microsoft.com

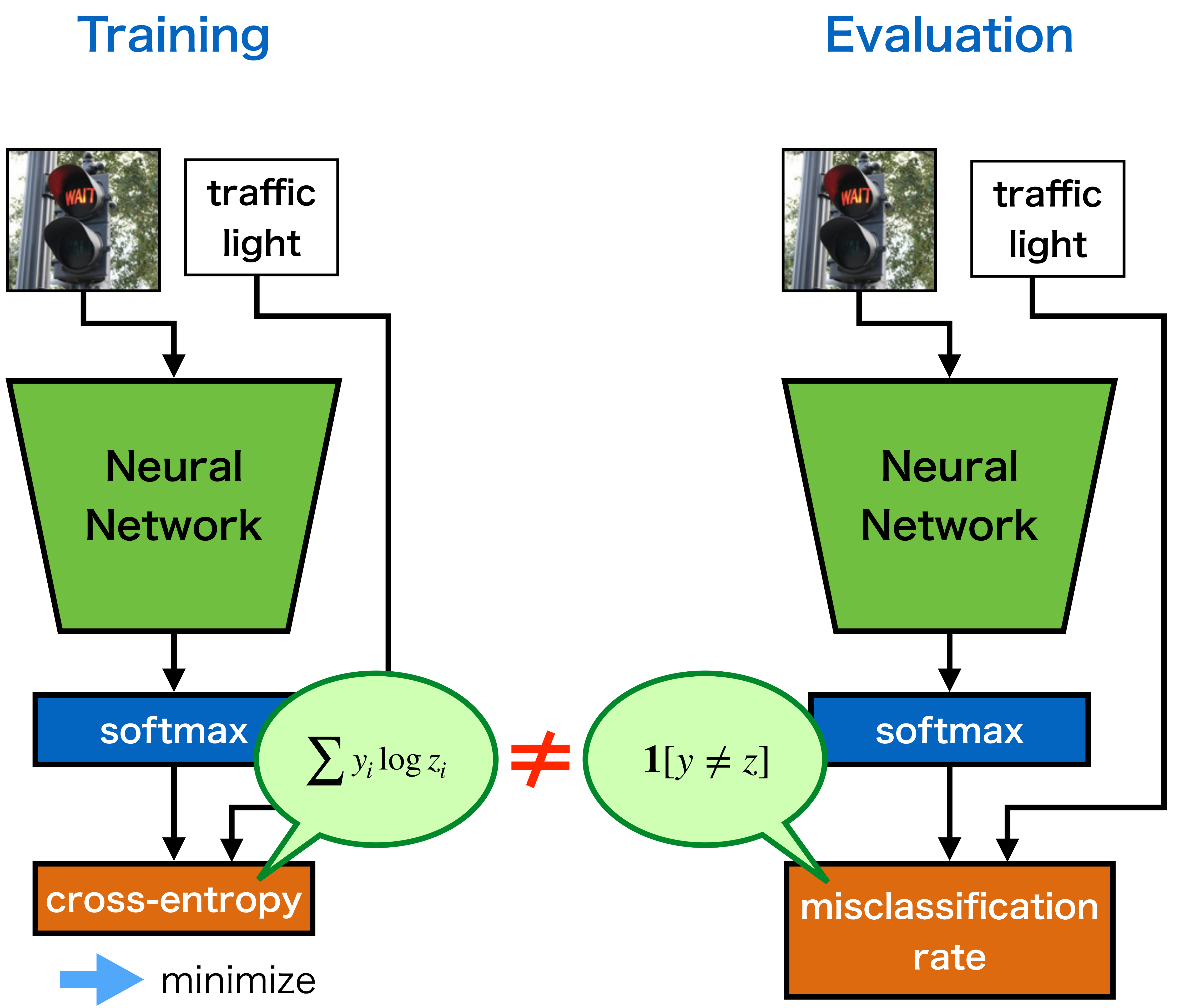






https://devblogs.nvidia.com/mocha-jl-deep-learning-julia/image1/

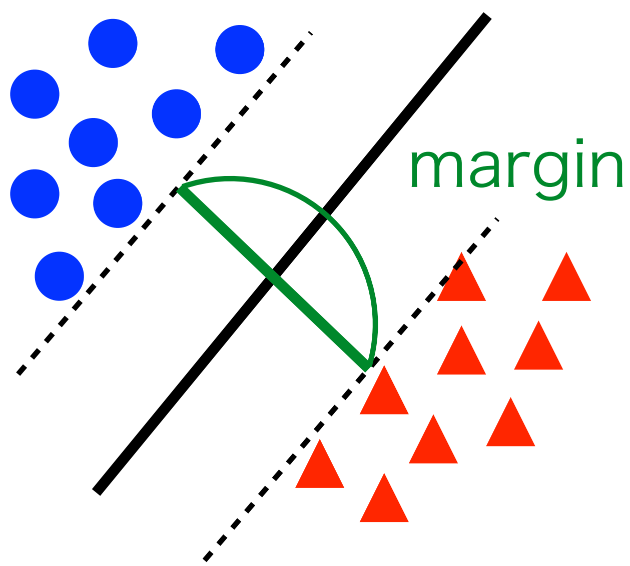

Training
feature (x)
label (y)
traffic light
Neural Network
softmax
cross-entropy
minimize
Distance of label and prediction
Prediction
feature (x)
Neural Network
softmax
traffic light?


Training
Evaluation
traffic light
traffic light
Neural Network
Neural Network
softmax
softmax
$\sum y_i \log z_i$
$\neq$
$\mathbf{1}[y \neq z]$
cross-entropy
misclassification rate
minimize

Machine Learning, 20, 273–297 (1995)

Support-Vector Networks

CORTINNA CORTES corinna@neural.att.com
VLADIMIR VAPNIK vlad@neural.att.com
AT&T Bell Labs., Holmdel, NJ 07733, USA



margin maximization

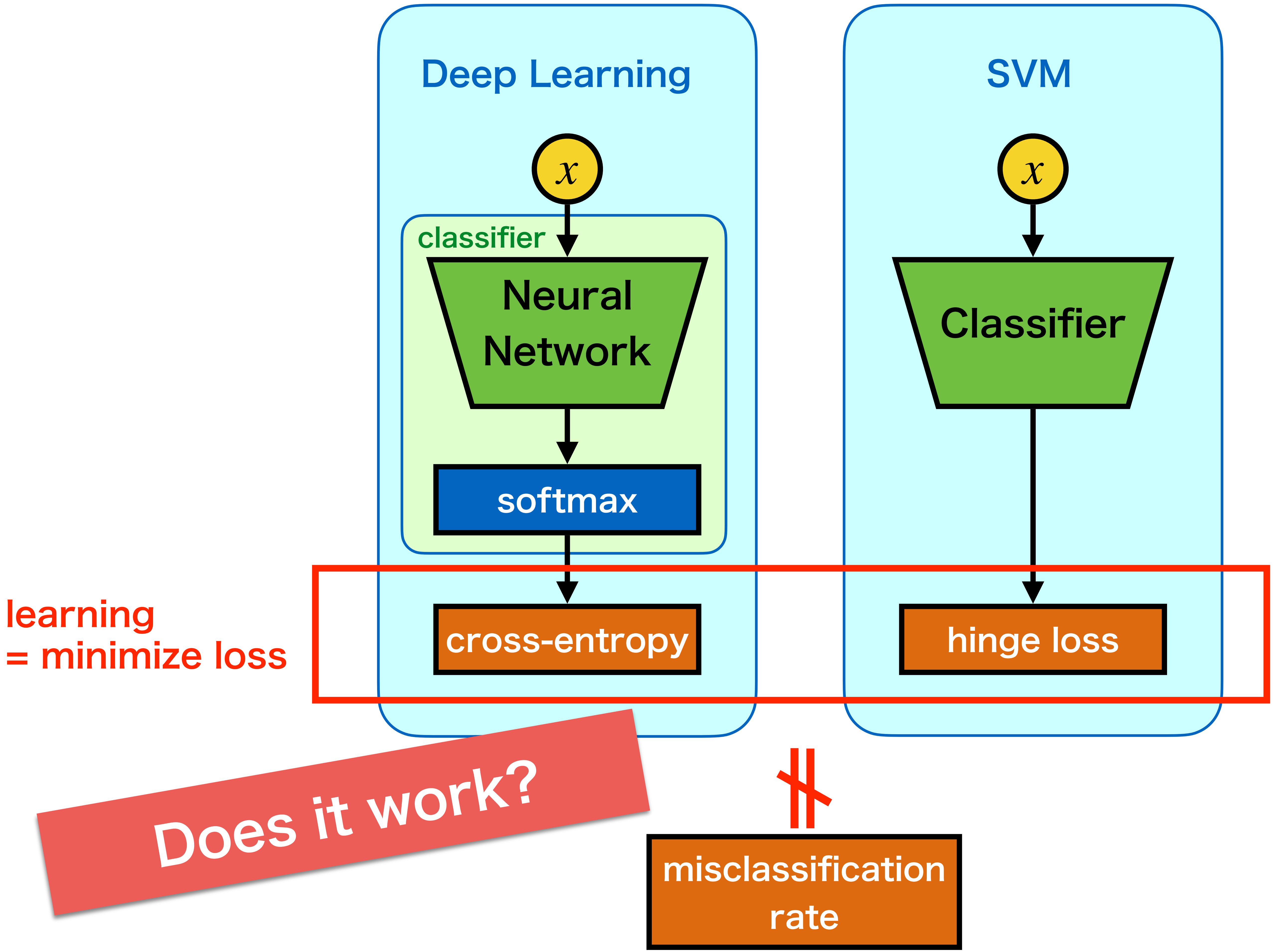
$=$

$$\min_{w,b} \sum_i \max\left\{0,\ 1 - y_i(w^\top x_i + b)\ \right\}$$

hinge loss minimization

$\neq$

misclassification rate

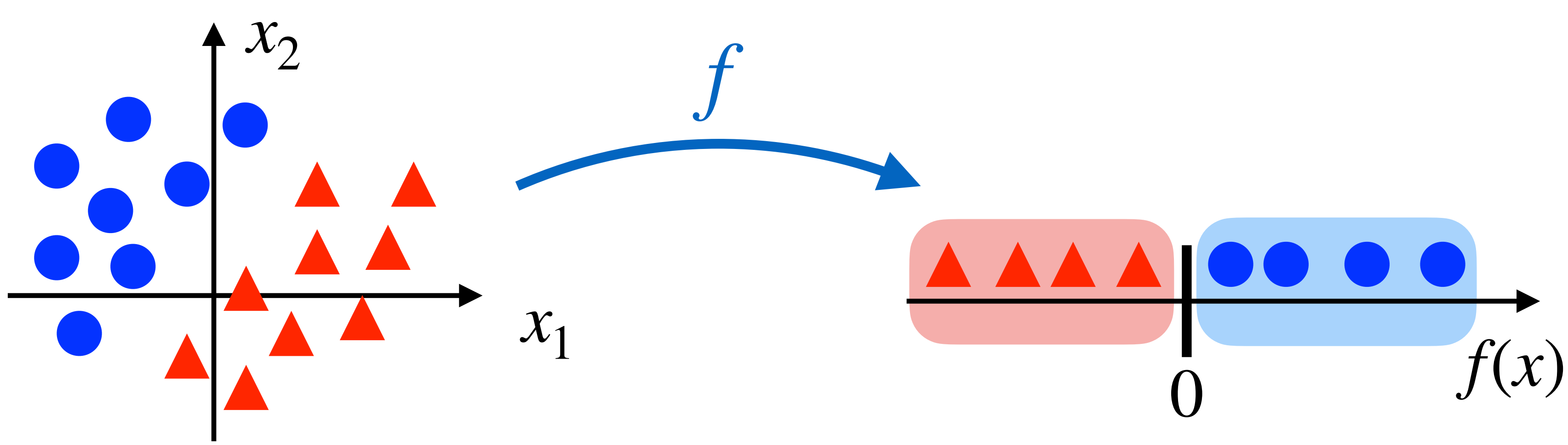


Deep Learning
x
classifier
Neural Network
softmax
cross-entropy
SVM
x
Classifier
hinge loss
learning
= minimize loss
Does it work?
$\nRightarrow$
misclassification rate

Background: Binary Classification

- Input
  - sample $\{(x_i, y_i)\}_{i=1}^n$: pair of feature $x_i \in \mathcal{X}$ and label $y_i \in \{\pm 1\}$
- Output
  - classifier $f : \mathcal{X} \to \mathbb{R}$
  - predict class by $\mathrm{sign}(f(\cdot))$
  - criteria: misclassification rate $R_{01}(f) = \mathbb{E}\left[\mathbf{1}[Y \neq \mathrm{sign}(f(X))]\right]$

1 if $Y \neq \mathrm{sign}(f(X))$,
0 if $Y = \mathrm{sign}(f(X))$



Loss function and Risk

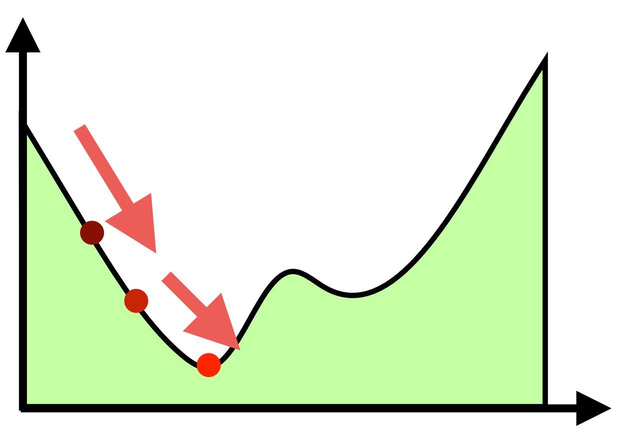
- Goal of classification: minimize misclassification rate

$$R_{01}(f) = \mathbb{E}\left[\mathbf{1}[Y \neq \mathrm{sign}(f(X))]\right]$$

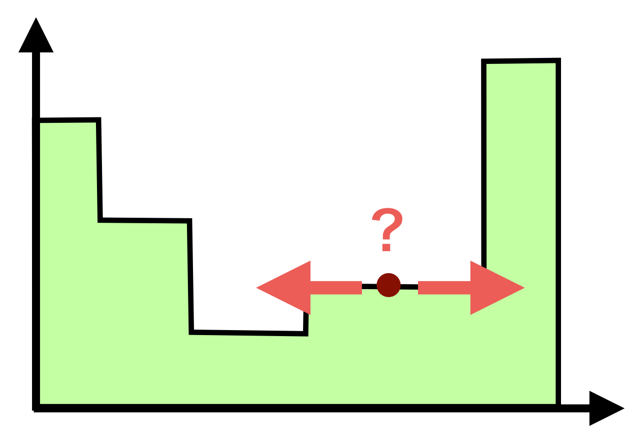
- Misclassification rate = expectation of 0-1 loss (0-1 risk)

$$\mathbf{1}[Y \neq \mathrm{sign}(f(X))] = \phi_{01}(Yf(X))$$

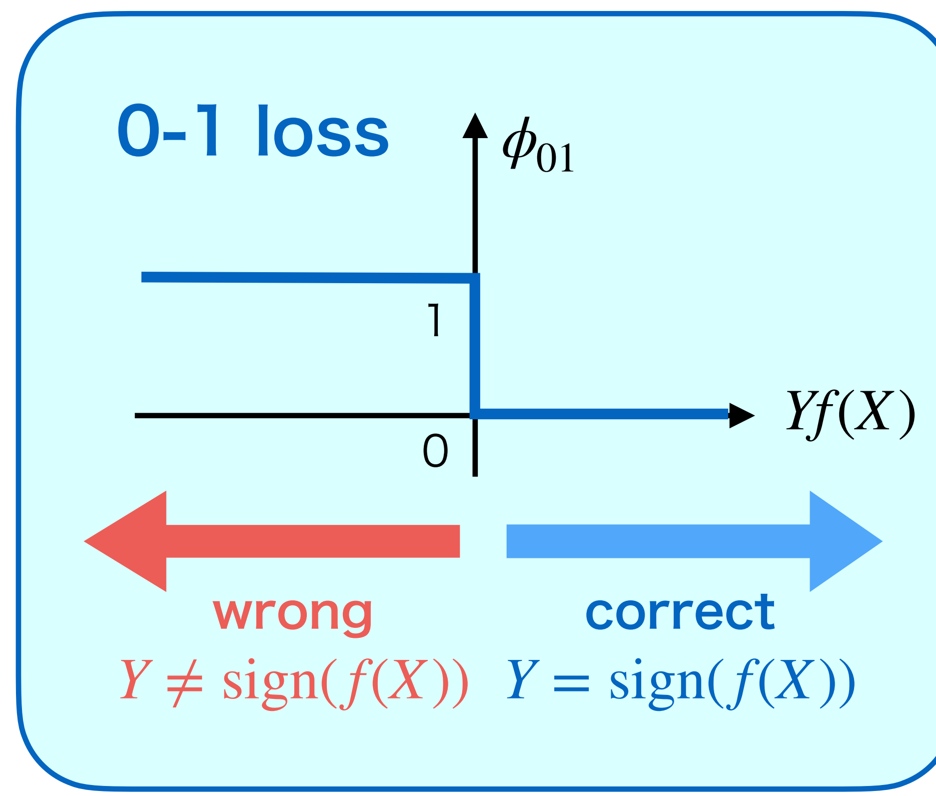
- Minimizing R_{01} is NP-hard [Feldman+ 2012]



minimization by gradient descent



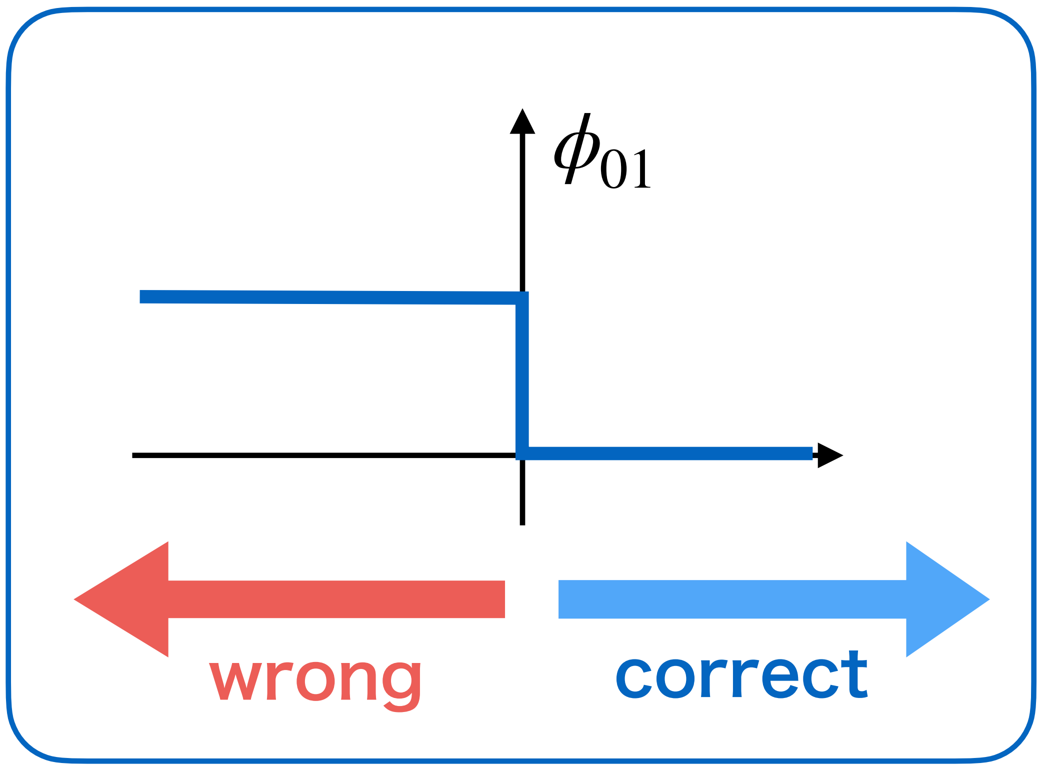
no gradient for discrete function



Feldman, V., Guruswami, V., Raghavendra, P., & Wu, Y. (2012). Agnostic learning of monomials by halfspaces is hard. *SIAM Journal on Computing*, *41*(6), 1558-1590.

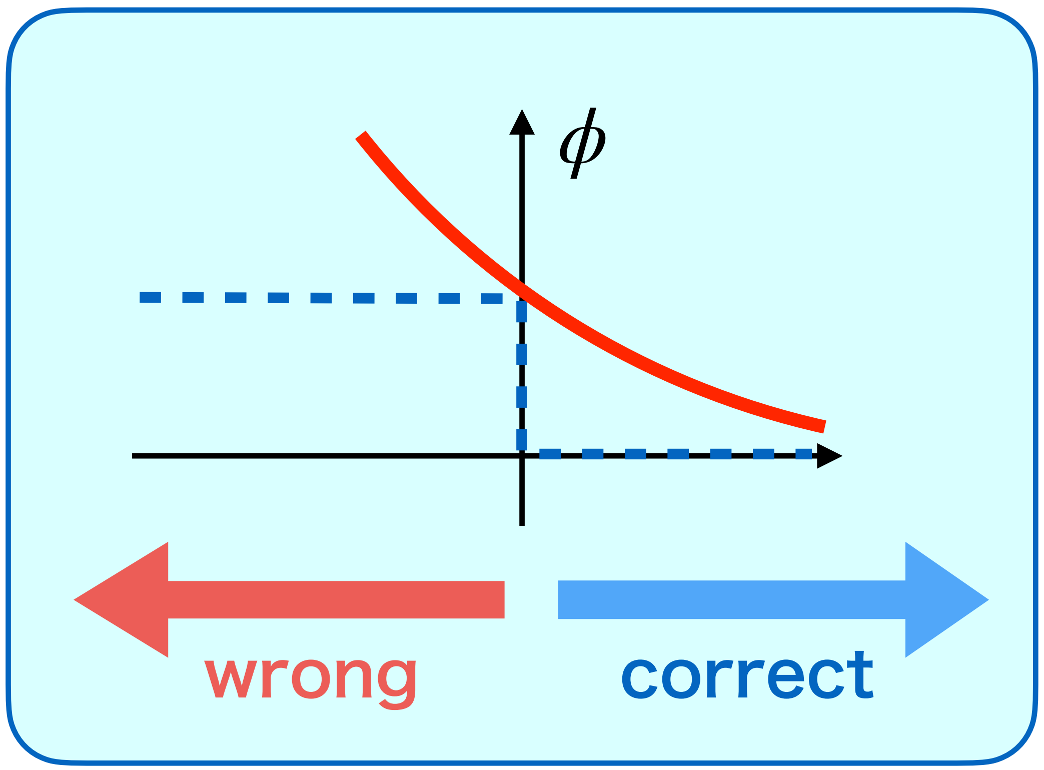
Target Loss vs. Surrogate Loss

Target loss (0-1 loss)



- Final learning criterion
- Hard to optimize
  - nonconvex, no gradient

Surrogate loss



- Different from target loss
- Easily-optimizable criterion
  - usually convex, smooth

Elements of Learning Theory

(empirical)
surrogate risk

$$\hat{R}_\phi(f) = \frac{1}{n}\sum_{i=1}^{n} \phi(y_i f(x_i))$$

Generalization theory:
If model is not too complicated,
then converges (roughly speaking)

(population)
surrogate risk

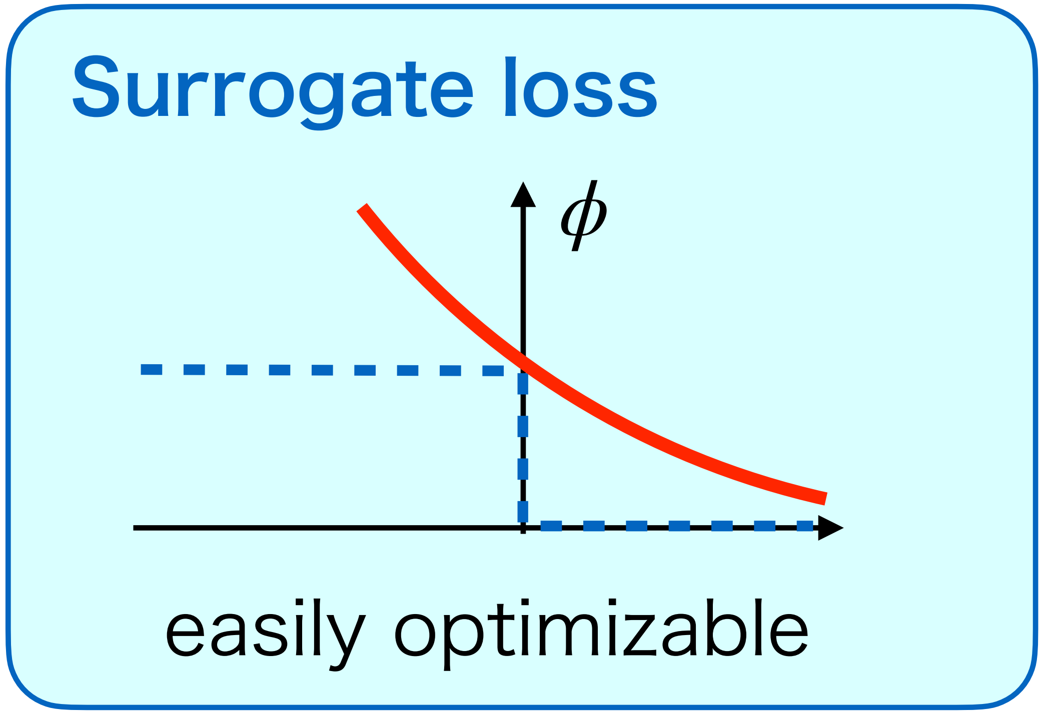
$$R_\phi(f) = \mathbb{E}[\phi(Yf(X))]$$

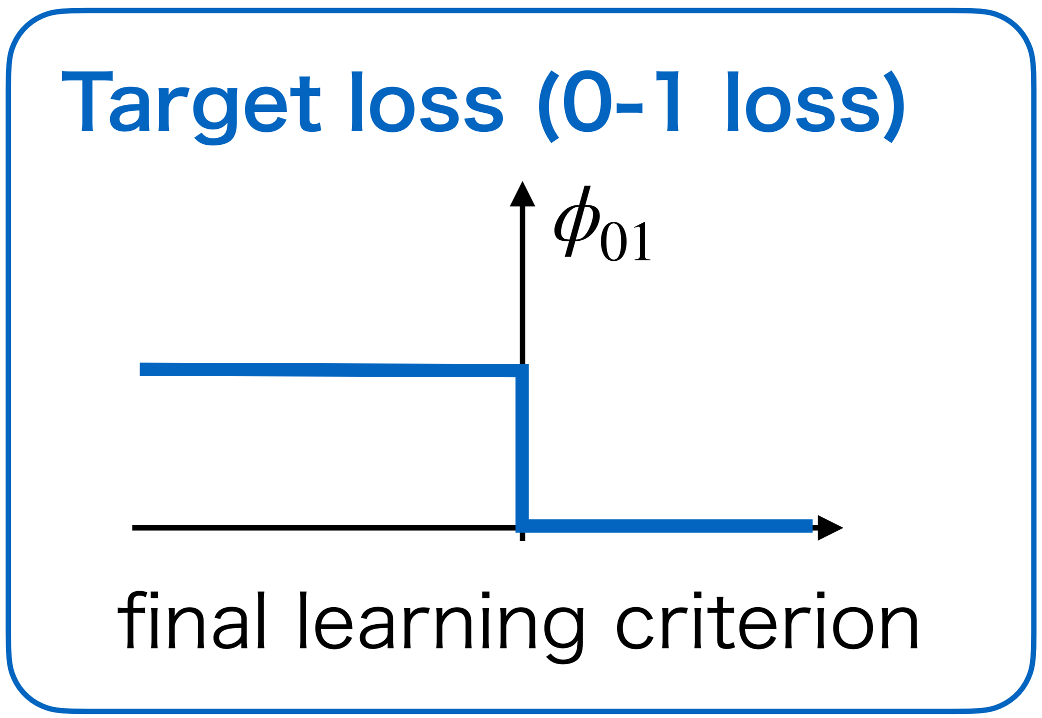
Key ingredient:
Calibration theory for
loss functions

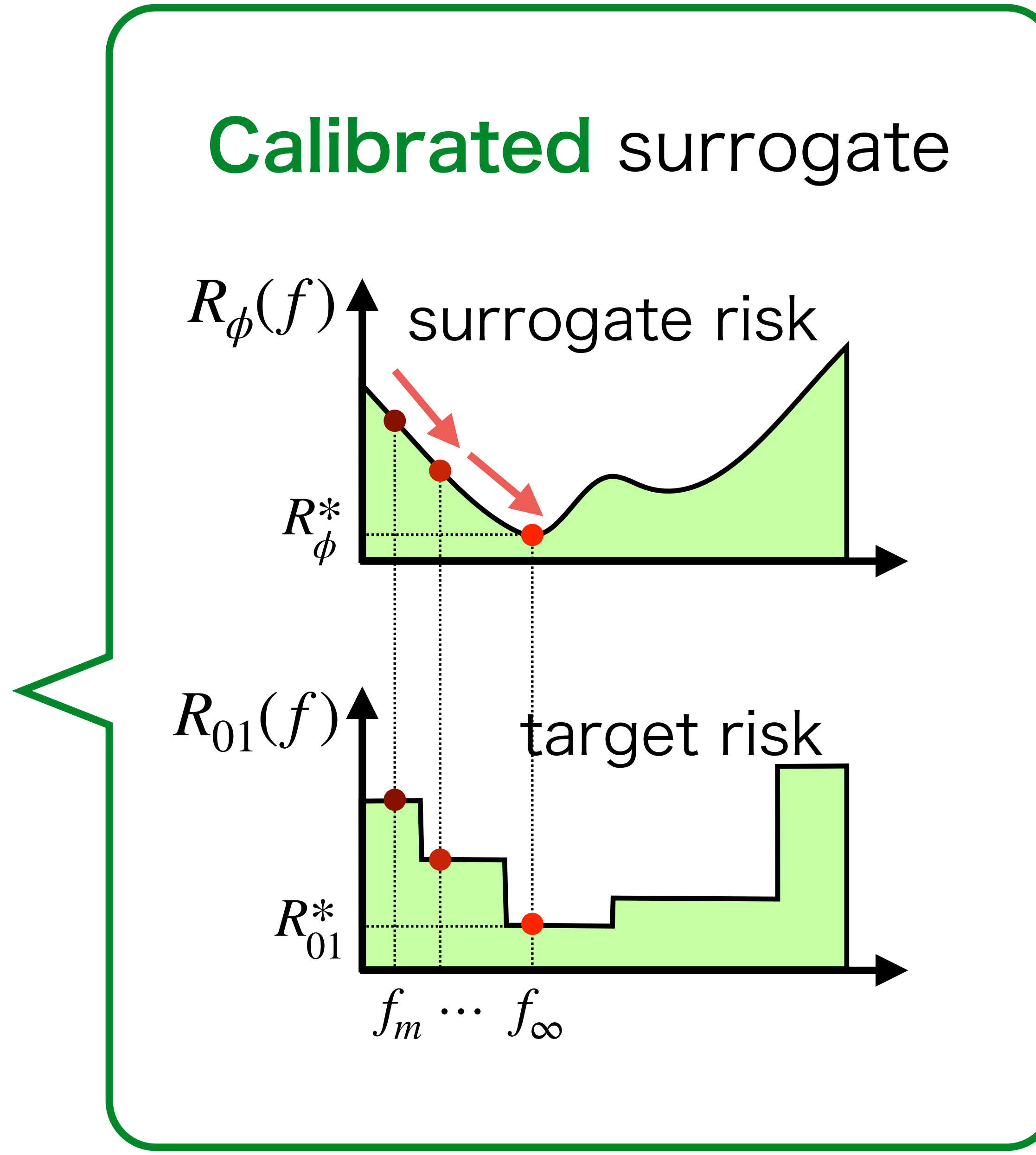
target risk

$$R_{01}(f) = \mathbb{E}[\phi_{01}(Yf(X))]$$

What surrogate is desirable?







$$R_\phi(f_m) \overset{m\to\infty}{\to} R_\phi^* \implies R_{01}(f_m) \overset{m\to\infty}{\to} R_{01}^*$$

How to check risk convergence?

[Steinwart 2007]

Definition. ϕ is ψ-**calibrated** for a target loss ψ if for any $\varepsilon > 0$, there exists $\delta > 0$ such that for all f,

$$\underbrace{R_\phi(f) - R_\phi^*}_{\text{surrogate (excess) risk}} < \delta \implies \underbrace{R_\psi(f) - R_\psi^*}_{\text{target (excess) risk}} < \varepsilon.$$

Idea: write δ as function of ε (by using contraposition)

Definition. (calibration function)

$$\delta(\varepsilon) = \inf_f \underbrace{R_\phi(f) - R_\phi^*}_{\text{surrogate (excess) risk}} \quad \text{s.t.} \quad \underbrace{R_\psi(f) - R_\psi^*}_{\text{target (excess) risk}} \geq \varepsilon$$

If $\delta(\varepsilon) > 0$ for all $\varepsilon > 0$, surrogate is calibrated!

Steinwart, I. (2007). How to compare different loss functions and their risks. *Constructive Approximation*, *26*(2), 225-287.

Main Tool: Calibration Function

Definition. (calibration function)

$$\delta(\varepsilon) = \inf_{f} \; R_\phi(f) - R_\phi^* \quad \text{s.t.} \quad R_\psi(f) - R_\psi^* \geq \varepsilon$$

surrogate (excess) risk　　target (excess) risk

- Provides **iff condition**
  - ψ-calibrated $\iff \delta(\varepsilon) > 0$ for all $\varepsilon > 0$
- Provides **excess risk bound**
  - ψ-calibrated $\implies R_\psi(f) - R_\psi^* \leq (\delta^{**})^{-1}\left(R_\phi(f) - R_\phi^*\right)$

target excess risk　　monotonically increasing　　surrogate excess risk

δ^{**}: biconjugate of δ

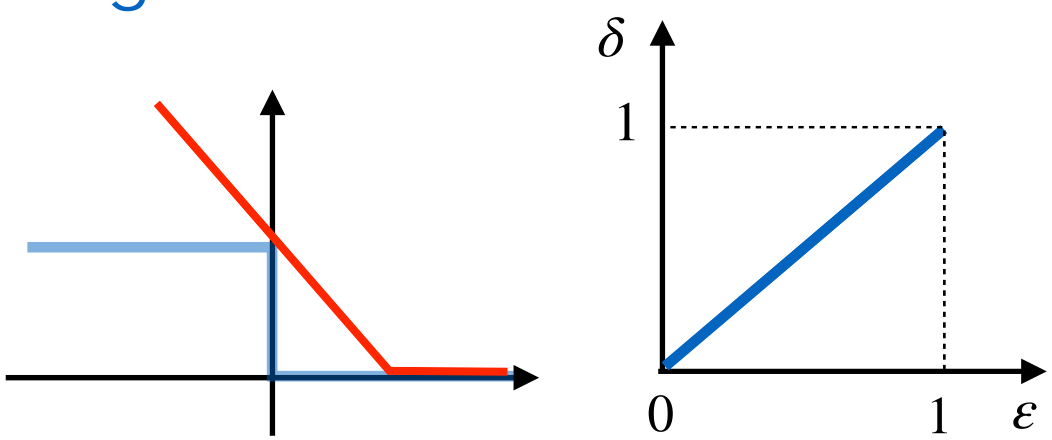
Example: Binary Classification (ϕ_{01})

[Bartlett+ 2006]

Theorem. If surrogate ϕ is convex, it is ϕ_{01}-calibrated iff

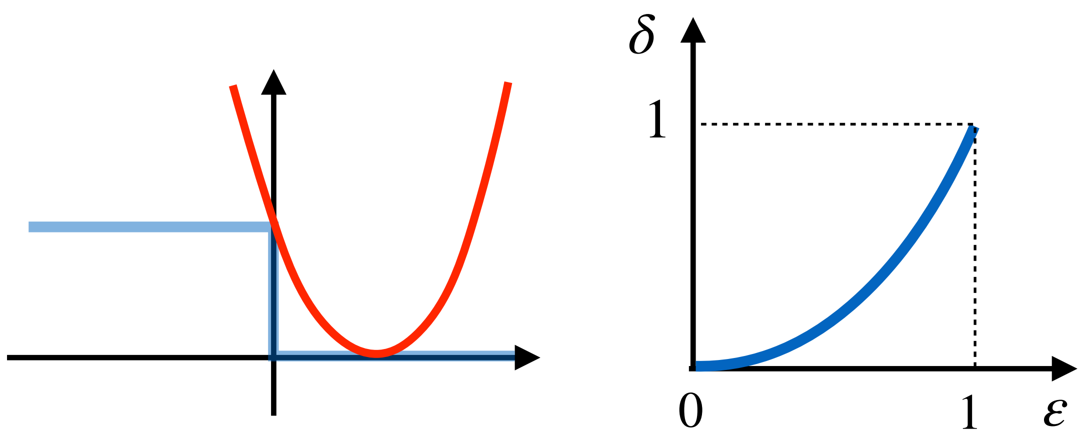
- differentiable at 0
- $\phi'(0) < 0$

hinge loss



$\phi(\alpha) = [1 - \alpha]_+$ $\delta(\varepsilon) = \varepsilon$

squared loss

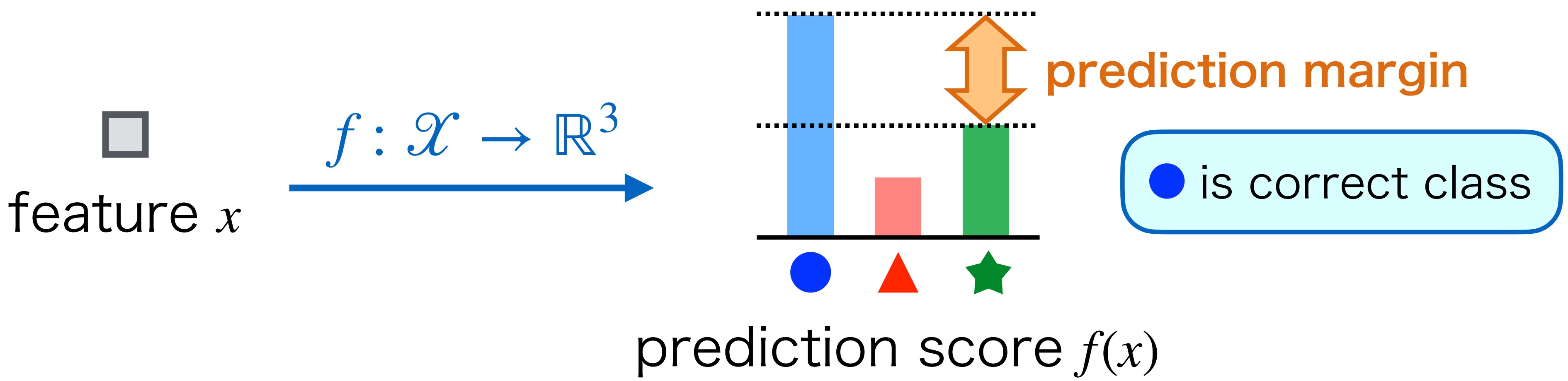


$\phi(\alpha) = (1 - \alpha)^2$ $\delta(\varepsilon) = \varepsilon^2$

P. L. Bartlett, M. I. Jordan, & J. D. McAuliffe. (2006).
Convexity, classification, and risk bounds. *Journal of the American Statistical Association*, 101(473), 138-156.

Counterintuitive Result

- e.g. multi-class classification $\Rightarrow$ maximize prediction margin



Crammer-Singer loss [Crammer & Singer 2001]

$\max\{0, 1 -$ pred. margin$\}$

one of multi-class extensions of hinge loss

Crammer-Singer loss is not calibrated to 0-1 loss !

(similar extension of logistic loss is calibrated)

[Zhang 2004]

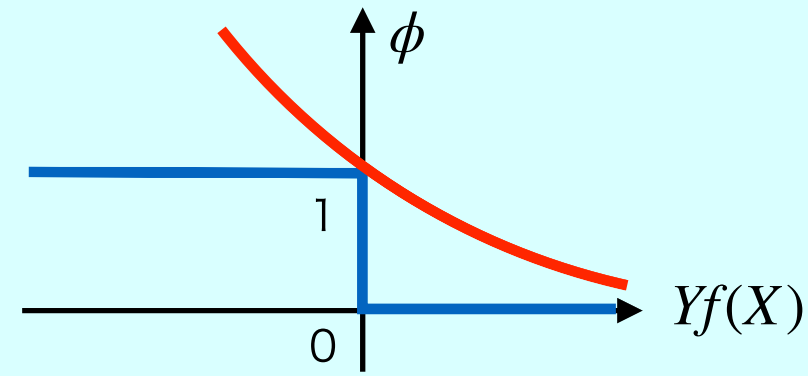
Crammer, K., & Singer, Y. (2001). On the algorithmic implementation of multiclass kernel-based vector machines. *Journal of machine learning research*, *2*(Dec), 265-292

Zhang, T. (2004). Statistical analysis of some multi-category large margin classification methods. *Journal of Machine Learning Research*, *5*(Oct), 1225-1251.

Summary: Calibration Theory

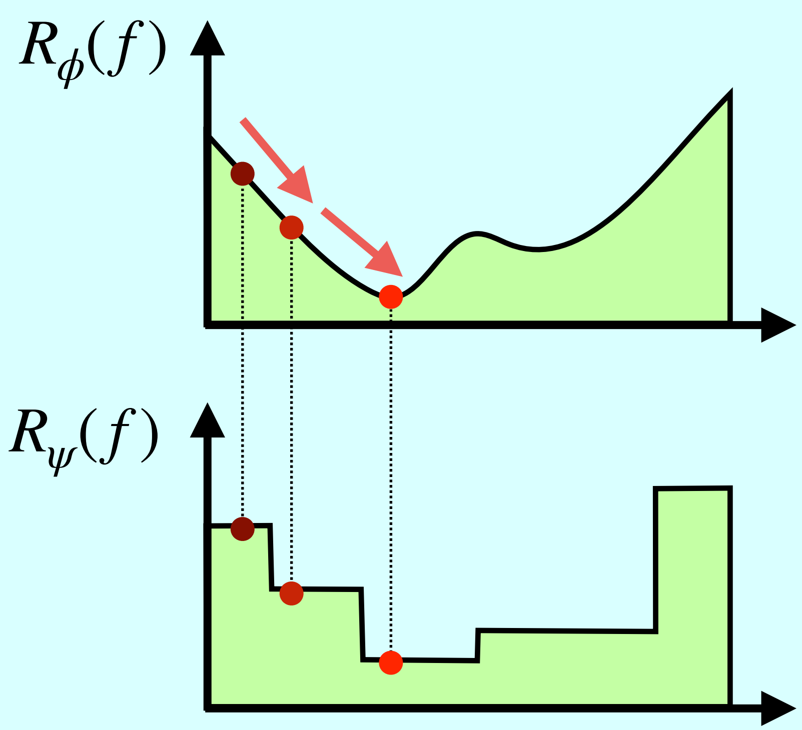
Surrogate vs. Target loss

Target loss is often hard to optimize
⇒ replace with **surrogate** loss



Calibrated Surrogate

leading to minimization of target



Binary Classification

Hinge, logistic is calibrated
Calibrated iff $\phi'(0) < 0$

Multi-class Classification

CS-loss (MC-hinge loss) is not calibrated!

cross-entropy is calibrated (omitted)

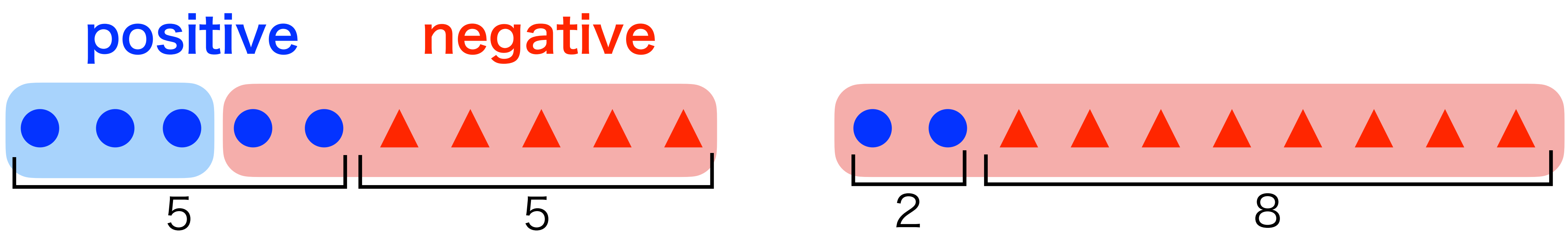
Stringent justification of surrogate loss!

When target is not 0-1 loss

H. Bao and M. Sugiyama.
Calibrated Surrogate Maximization of Linear-fractional Utility in Binary Classification. In *AISTATS*, 2020.

Is accuracy appropriate?

- Our focus: **binary classification**



seemingly sensible classifier

unreasonable classifier

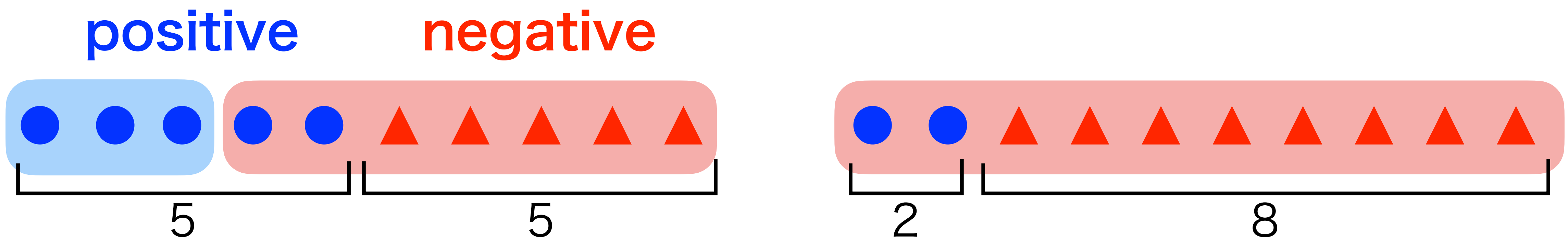
accuracy: **0.8**

accuracy: **0.8**

Accuracy can’t detect unreasonable classifiers under **class imbalance**!

Is accuracy appropriate?

- F-measure is more appropriate under **class imbalance**



accuracy: **0.8**
F-measure: **0.75**

accuracy: **0.8**
F-measure: **0**

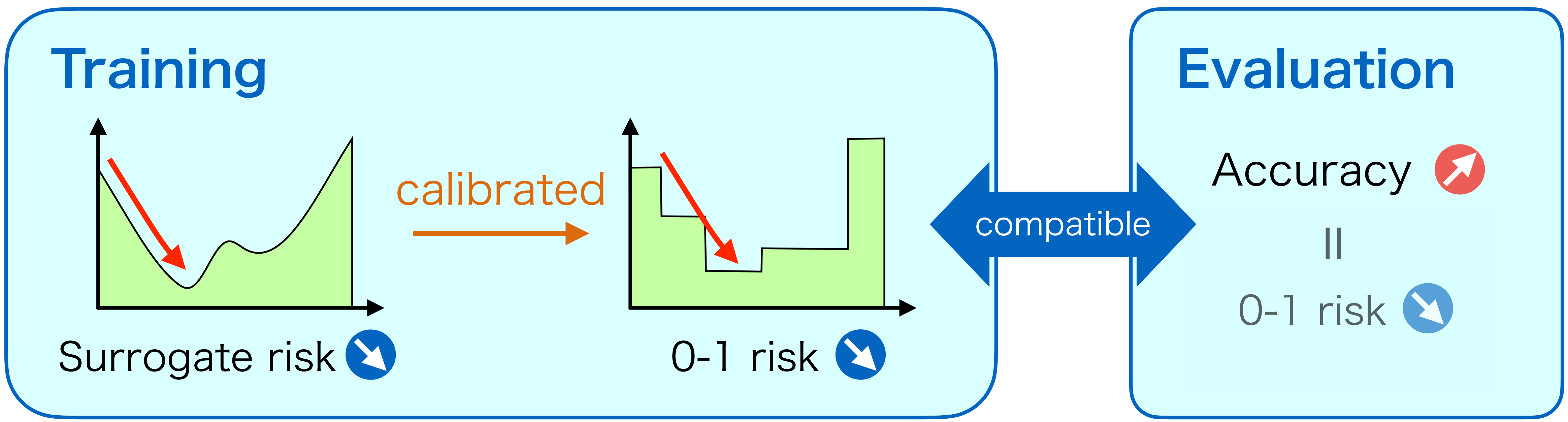
F-measure $$F_1 = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

$$\mathrm{TP} = \mathbb{E}_{X,Y=+1}[1_{\{f(X)>0\}}] \qquad \mathrm{TN} = \mathbb{E}_{X,Y=-1}[1_{\{f(X)<0\}}]$$

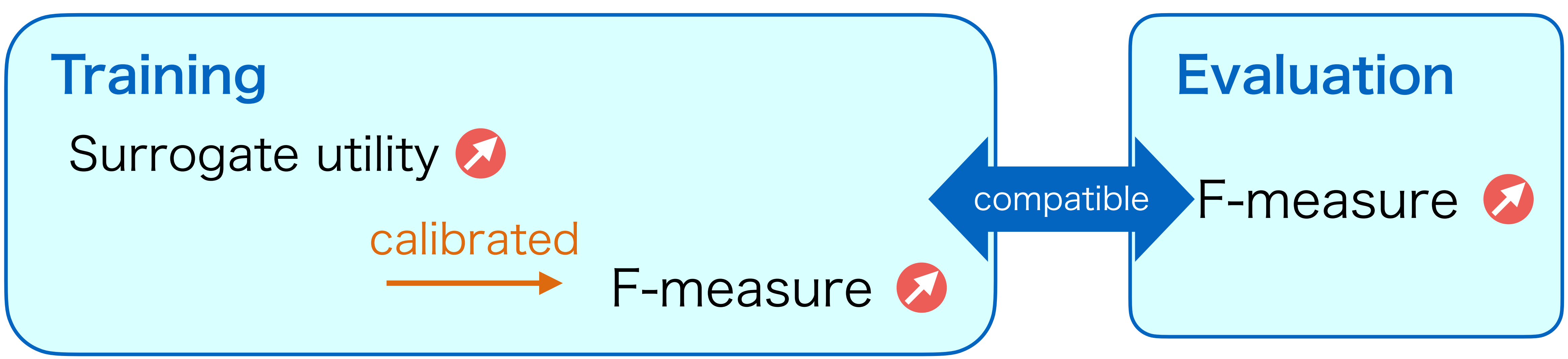
$$\mathrm{FP} = \mathbb{E}_{X,Y=-1}[1_{\{f(X)>0\}}] \qquad \mathrm{FN} = \mathbb{E}_{X,Y=+1}[1_{\{f(X)<0\}}]$$

Training and Evaluation

- Usual training with accuracy



- Training with accuracy but evaluating with F-measure



Not only F_1, but many others

Q. Can we handle in the same way?

Accuracy

$$\mathrm{Acc} = \mathrm{TP} + \mathrm{TN}$$

Weighted Accuracy

$$\mathrm{WAcc} = \frac{w_1\mathrm{TP} + w_2\mathrm{TN}}{w_1\mathrm{TP} + w_2\mathrm{TN} + w_3\mathrm{FP} + w_4\mathrm{FN}}$$

F-measure

$$F_1 = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

Balanced Error Rate

$$\mathrm{BER} = \frac{1}{\pi}\mathrm{FN} + \frac{1}{1-\pi}\mathrm{FP}$$

Gower-Legendre index

$$\mathrm{GLI} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \alpha(\mathrm{FP} + \mathrm{FN}) + \mathrm{TN}}$$

Jaccard index

$$\mathrm{Jac} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

Unification of Metrics

Note:

$\mathrm{TN} = \mathbb{P}(Y = -1) - \mathrm{FP}$

$\mathrm{FN} = \mathbb{P}(Y = +1) - \mathrm{TP}$

Actual Metrics

$$\mathrm{F}_1 = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

$$\mathrm{Jac} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

linear-fraction

$$U(f) = \frac{a_0\mathrm{TP} + b_0\mathrm{FP} + c_0}{a_1\mathrm{TP} + b_1\mathrm{FP} + c_1}$$

a_k, b_k, c_k : constants

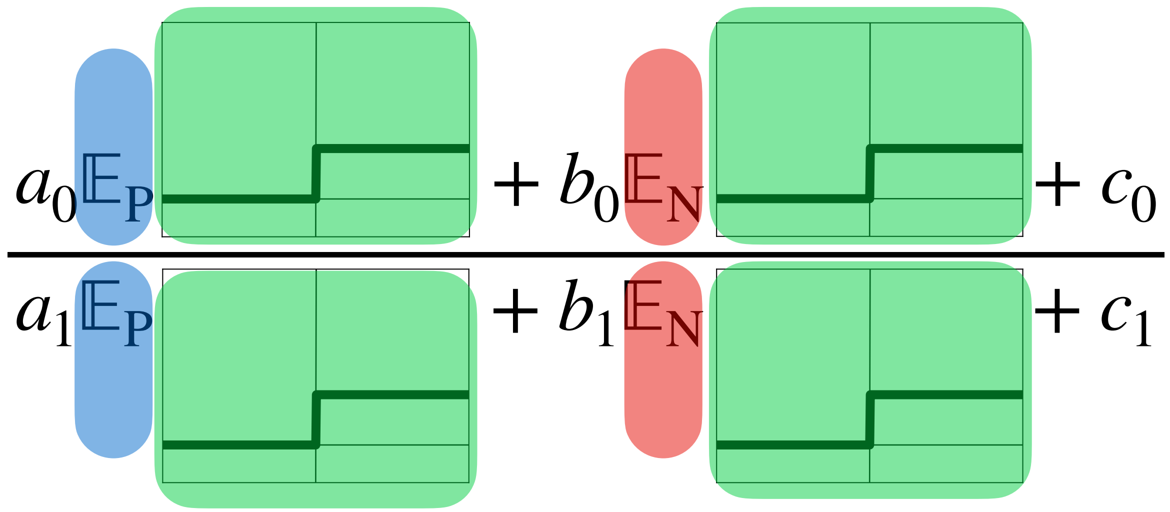
Unification of Metrics

linear-fraction

$$U(f) = \frac{a_0\mathrm{TP} + b_0\mathrm{FP} + c_0}{a_1\mathrm{TP} + b_1\mathrm{FP} + c_1}$$

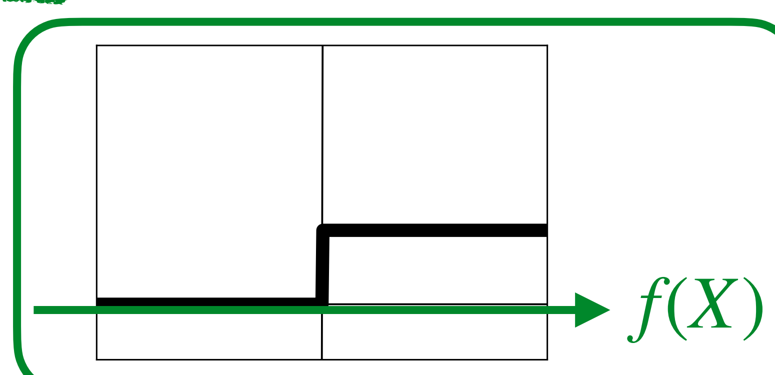
expectation divided by expecation

=



$$:= \frac{\mathbb{E}_X[W_0(f(X))]}{\mathbb{E}_X[W_1(f(X))]}$$

- TP, FP = expectation of 0/1-loss
  - TP $= \mathbb{E}_{X,Y=+1}\left[\mathbf{1}[f(X) > 0]\right]$
    positive data && positive prediction
  - FP $= \mathbb{E}_{X,Y=-1}\left[\mathbf{1}[f(X) > 0]\right]$
    negative data && positive prediction



Goal of This Talk

Given a metric (utility) $U(f) = \dfrac{a_0\text{TP} + b_0\text{FP} + c_0}{a_1\text{TP} + b_1\text{FP} + c_1}$

Q. How to optimize $U(f)$ directly?

- without estimating class-posterior probability

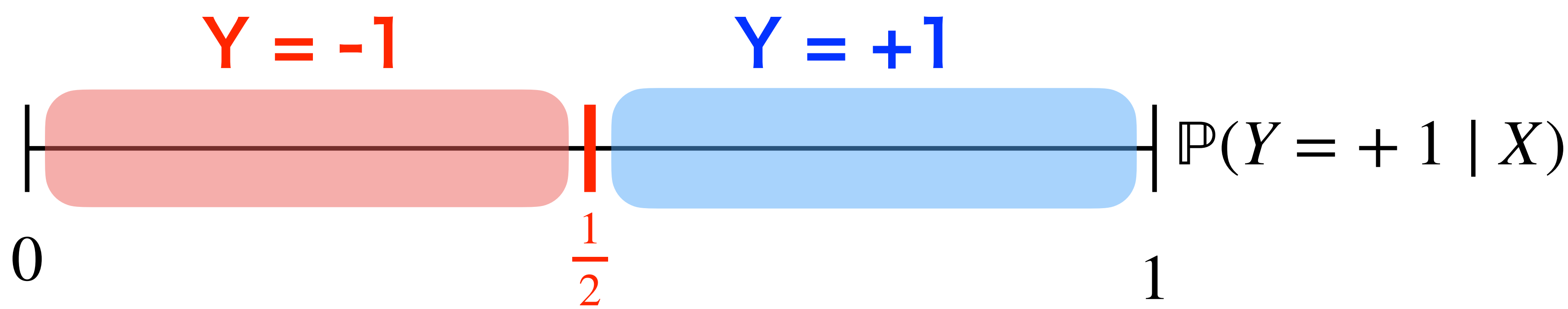
labeled sample $\{(x_i, y_i)\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} \mathbb{P}$ metric U	→	classifier $f : \mathcal{X} \to \mathbb{R}$ s.t. $U(f) = \sup_{f'} U(f')$

Related: Plug-in Classifier

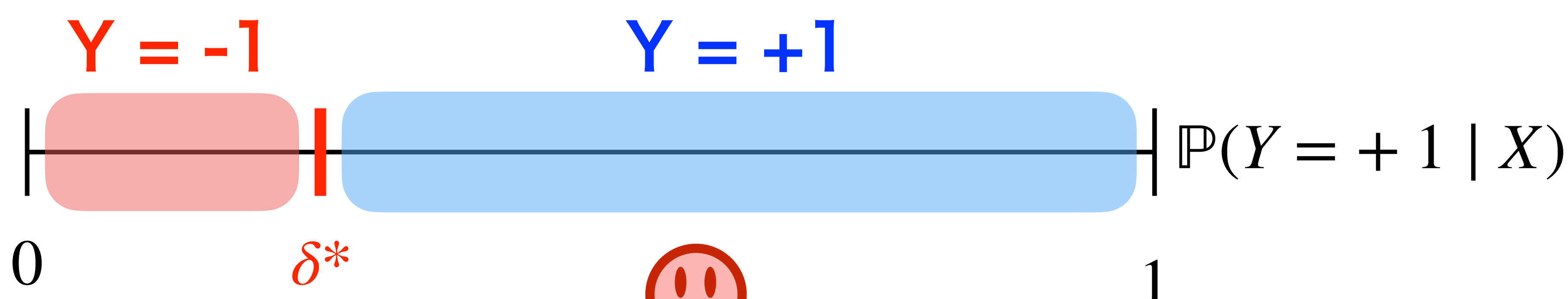
[Koyejo+ NIPS2014; Yan+ ICML2018]

- Estimating class-posterior probability is costly!

Bayes-optimal classifier (accuracy): $\mathbb{P}(Y=+1\,|\,x)-\frac{1}{2}$



Bayes-optimal classifier (general case): $\mathbb{P}(Y=+1\,|\,x)-\delta^*$



$\Rightarrow$ estimate $\boxed{\mathbb{P}(Y=+1\,|\,x)}$ and δ^* independently

O. O. Koyejo, N. Natarajan, P. K. Ravikumar, & I. S. Dhillon.
Consistent binary classification with generalized performance metrics. In *NIPS*, 2014.

B. Yan, O. Koyejo, K. Zhong, & P. Ravikumar.
Binary classification with Karmic, threshold-quasi-concave metrics. In *ICML*, 2018.

Convexity & Statistical Property

Q. How to make tractable surrogate?

Accuracy

tractable (convex)

$$R_\phi(f) = \mathbb{E}[\phi(Yf(X))]$$

calibrated

intractable

$$R_{01}(f) = \mathbb{E}[\phi_{01}(Yf(X))]$$

Linear-fractional Metrics

① tractable?

? ? ?

② calibrated?

intractable

$$U(f) = \frac{\mathbb{E}_X[W_0(f(X))]}{\mathbb{E}_X[W_1(f(X))]}$$

Non-concave, but quasi-concave

Idea: $\dfrac{\text{concave}}{\text{convex}}$ = quasi-concave

$\dfrac{f(x)}{g(x)}$ is quasi-concave

if f : concave, g : convex,

$f(x) \geq 0$ and $g(x) > 0$ for $\forall x$

(proof) Show $\{x \mid f/g \geq \alpha\}$ is convex.

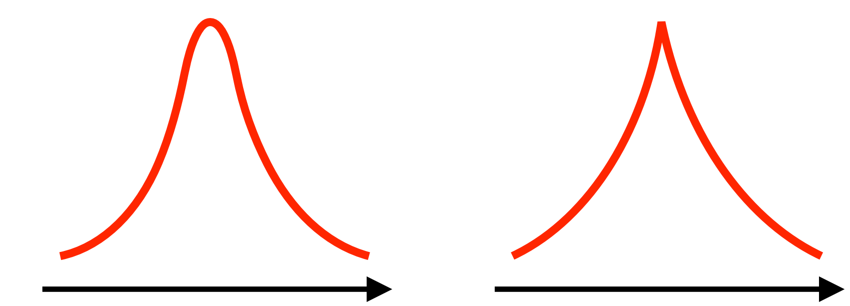
$$\frac{f(x)}{g(x)} \geq \alpha \Longleftrightarrow \underbrace{f(x) - \alpha g(x)}_{\text{concave}} \geq 0$$

NB: super-level set of concave func. is convex

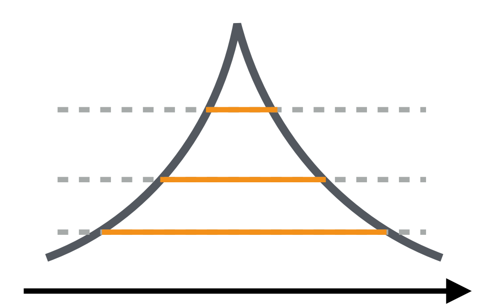
$\therefore \{x \mid f/g \geq \alpha\}$ is convex for $\forall \alpha \geq 0$

non-concave, but unimodal

⇒ efficiently optimized

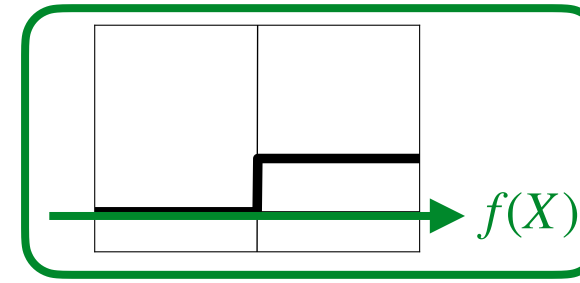


- quasi-concave ⊇ concave
- super-levels are convex



Surrogate Utility

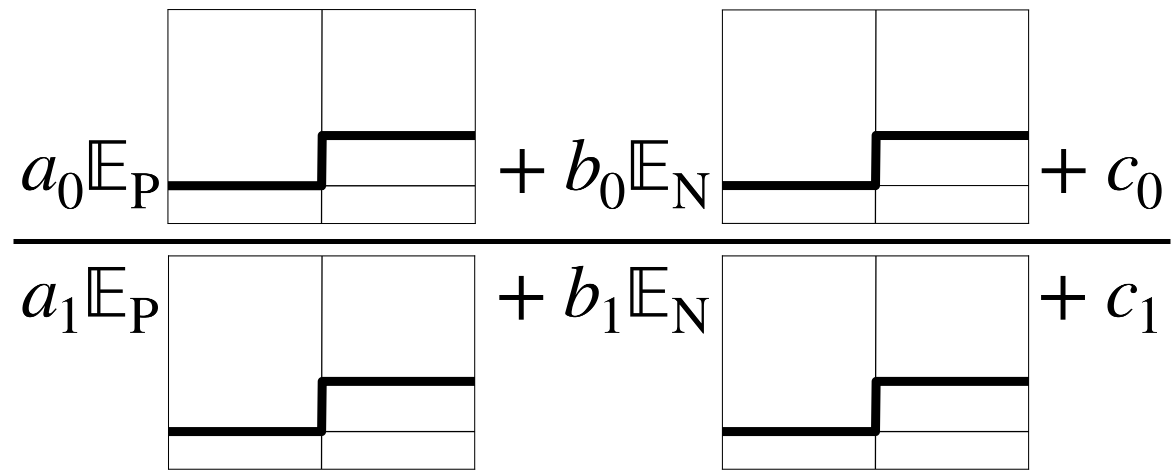
- Idea: bound true utility from below



linear-fraction

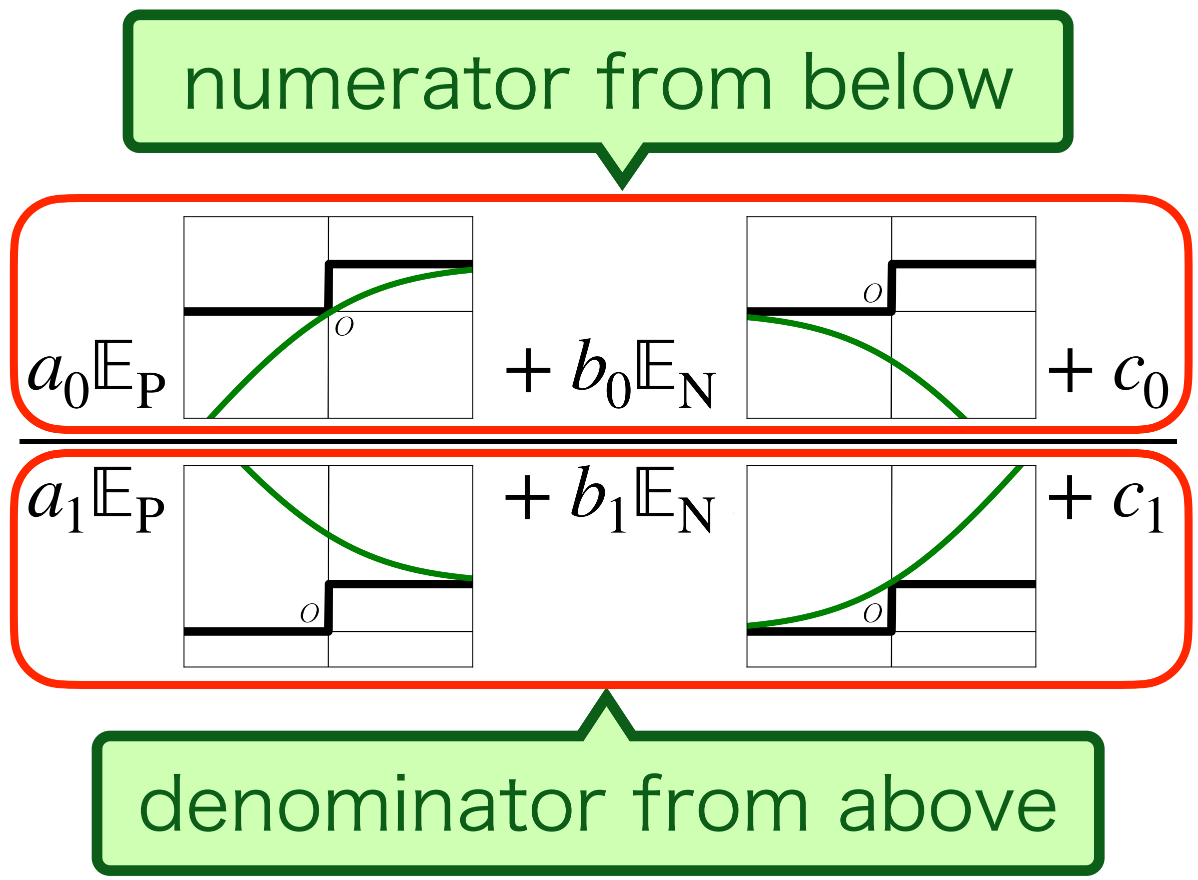
$$U(f) = \frac{a_0\text{TP} + b_0\text{FP} + c_0}{a_1\text{TP} + b_1\text{FP} + c_1}$$

=



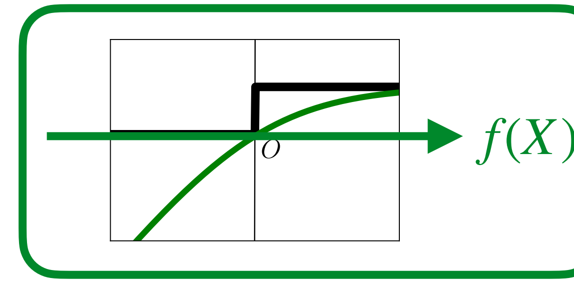
non-negative sum of concave
⇒ concave

≥



non-negative sum of convex
⇒ convex

Surrogate Utility

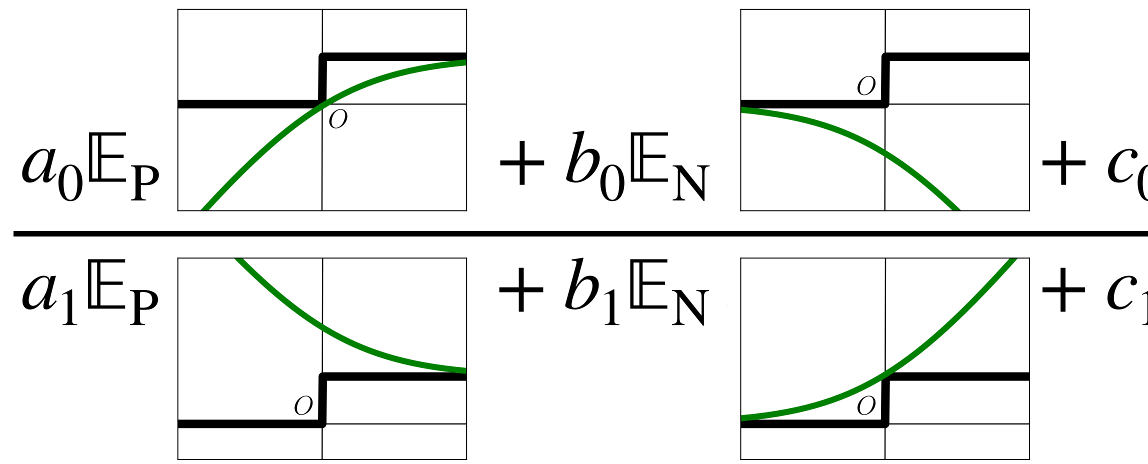


- Idea: bound true utility from below

linear-fraction

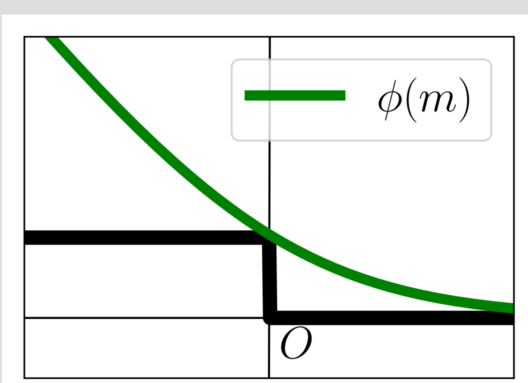
$$U(f) = \frac{a_0\mathrm{TP} + b_0\mathrm{FP} + c_0}{a_1\mathrm{TP} + b_1\mathrm{FP} + c_1}$$

$\geq$



$=$

surrogate loss

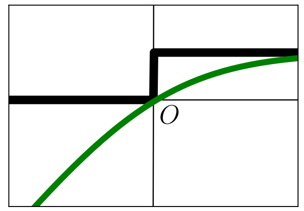
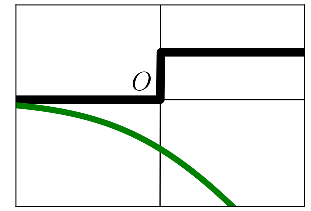
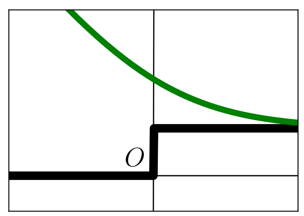
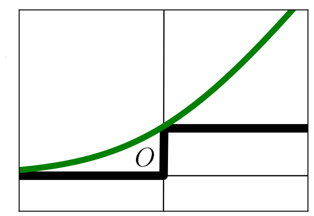
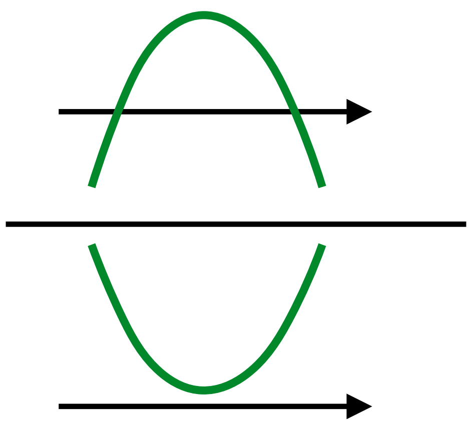


$$U_\phi(f) = \frac{a_0\mathbb{E}_\mathrm{P}\boxed{[1-\phi(f(X))]} + b_0\mathbb{E}_\mathrm{N}\boxed{[-\phi(-f(X))]} + c_0}{a_1\mathbb{E}_\mathrm{P}\boxed{[1+\phi(f(X))]} + b_1\mathbb{E}_\mathrm{N}\boxed{[\ \phi(-f(X))\ ]} + c_1}$$

$$:= \frac{\mathbb{E}[W_{0,\phi}]}{\mathbb{E}[W_{1,\phi}]}$$ **: Surrogate Utility**

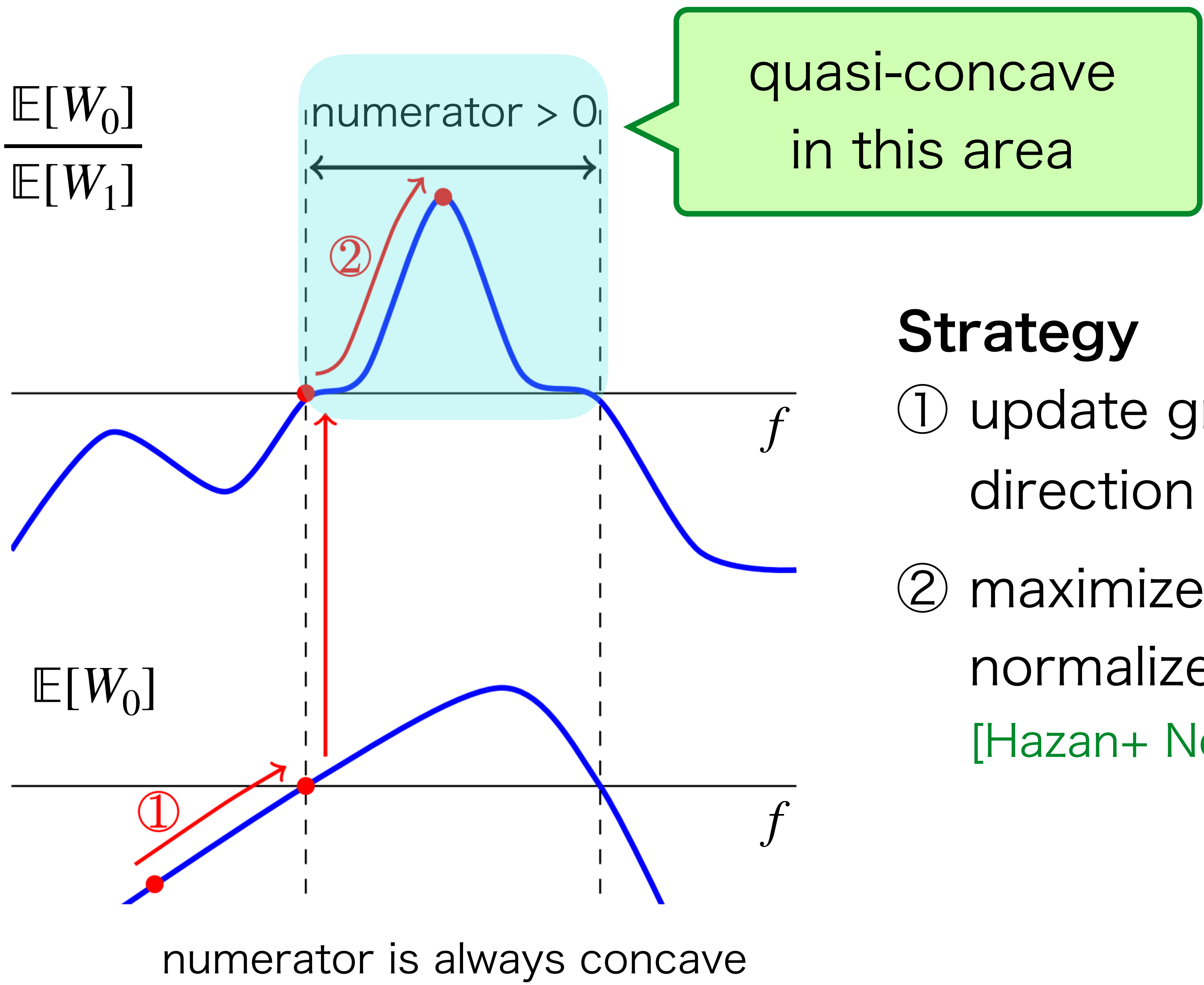
Hybrid Optimization Strategy

$$U_\phi(f) = \frac{a_0 \mathbb{E}_\mathrm{P} + b_0 \mathbb{E}_\mathrm{N} + c_0}{a_1 \mathbb{E}_\mathrm{P} + b_1 \mathbb{E}_\mathrm{N} + c_1} =$$

- Note: numerator can be negative
  - U_ϕ isn't quasi-concave only if numerator < 0
  - make numerator positive first (concave), then maximize fractional form (quasi-concave)

Hybrid Optimization Strategy



Strategy

① update gradient-ascent direction while $\mathbb{E}[W_0] < 0$

② maximize fraction by normalized-gradient ascent [Hazan+ NeurIPS2015]

Hazan, E., Levy, K., & Shalev-Shwartz, S. (2015). Beyond convexity: Stochastic quasi-convex optimization. In *Advances in Neural Information Processing Systems* (pp. 1594-1602).

Convexity & Statistical Property

Q. How to make surrogate calibrated?

Accuracy

tractable (convex)

$$R_\phi(f) = \mathbb{E}[\phi(Yf(X))]$$

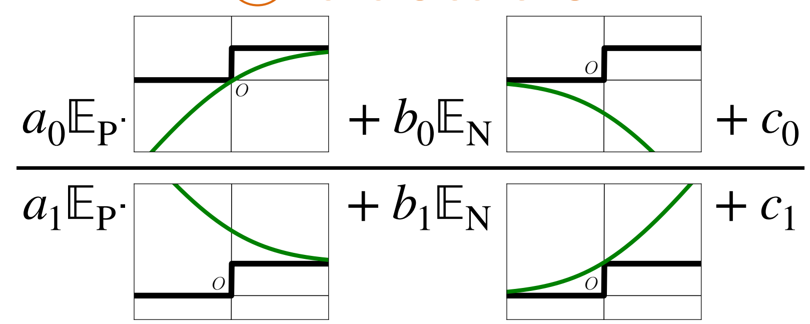
calibrated

intractable

$$R_{01}(f) = \mathbb{E}[\phi_{01}(Yf(X))]$$

Linear-fractional Metrics

① tractable



② calibrated?

intractable

$$U(f) = \frac{\mathbb{E}_X[W_0(f(X))]}{\mathbb{E}_X[W_1(f(X))]}$$

Special Case: F1-measure

Theorem

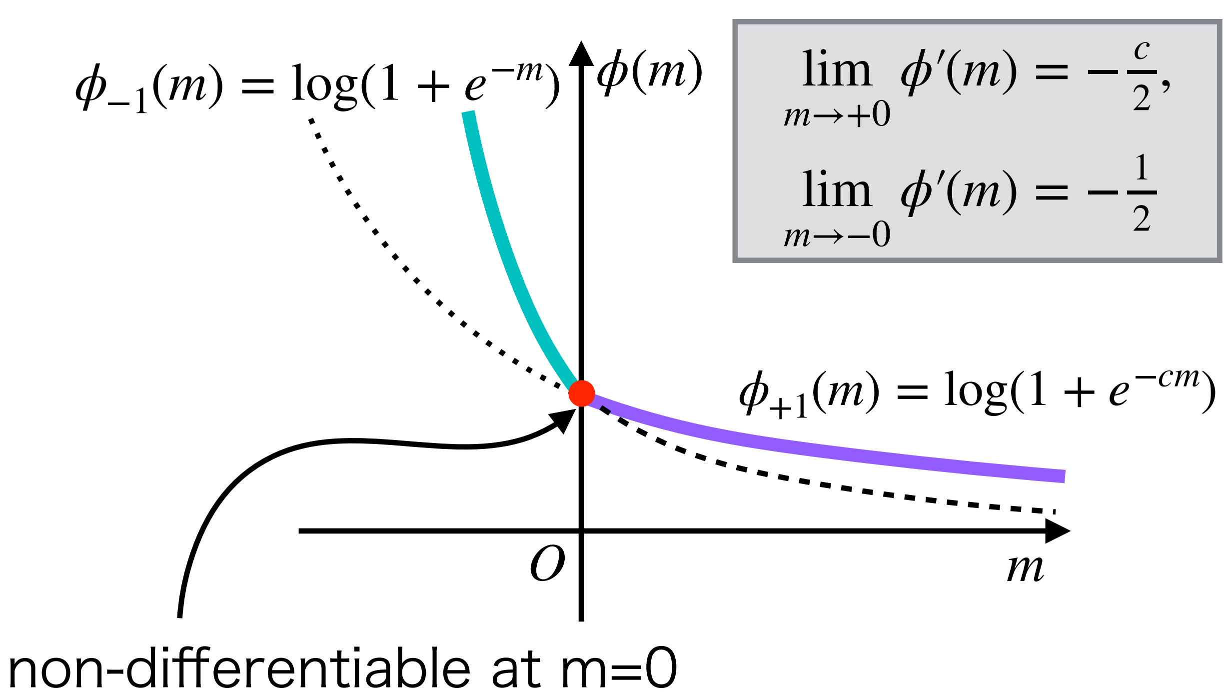
$$U_\phi(f_n) \overset{n\to\infty}{\to} 1 \Longrightarrow U(f_n) \overset{n\to\infty}{\to} 1 \quad \forall\{f_n\}$$

if ϕ satisfies

- $\exists c \in (0,1)$ s.t. $\sup_f U_\phi(f) \geq \frac{2c}{1-c}$, $\lim_{m\to+0}\phi'(m) \geq c \lim_{m\to-0}\phi'(m)$
- ϕ is non-increasing
- ϕ is convex

Note: informal

- Example



Intuition:

trade off TP and FP

by gradient steepness

Experiment: F_1-measure

(F_1-measure)	Proposed		Baselines		
Dataset	U-GD	U-BFGS	ERM	W-ERM	Plug-in
adult	0.617 (101)	0.660 (11)	0.639 (51)	0.676 (18)	**0.681 (9)**
australian	**0.843 (41)**	**0.844 (45)**	0.820 (123)	0.814 (116)	0.827 (51)
breast-cancer	**0.963 (31)**	**0.960 (32)**	0.950 (37)	0.948 (44)	0.953 (40)
cod-rna	0.802 (231)	0.594 (4)	0.927 (7)	0.927 (6)	**0.930 (2)**
diabetes	**0.834 (32)**	**0.828 (31)**	0.817 (50)	0.821 (40)	0.820 (42)
fourclass	**0.638 (70)**	**0.638 (64)**	0.601 (124)	0.591 (212)	0.618 (64)
german.numer	0.561 (102)	**0.580 (74)**	0.492 (188)	0.560 (107)	**0.589 (73)**
heart	**0.796 (101)**	**0.802 (99)**	**0.792 (80)**	0.764 (151)	0.764 (137)
ionosphere	**0.908 (49)**	**0.901 (43)**	0.883 (104)	0.842 (217)	**0.897 (54)**
madelon	**0.666 (19)**	0.632 (67)	0.491 (293)	0.639 (110)	**0.663 (24)**
mushrooms	1.000 (1)	0.997 (7)	**1.000 (1)**	1.000 (2)	0.999 (4)
phishing	0.937 (29)	**0.943 (7)**	**0.944 (8)**	0.940 (12)	**0.944 (8)**
phoneme	**0.648 (27)**	0.559 (22)	0.530 (201)	0.616 (135)	0.633 (35)
skin_nonskin	0.870 (3)	0.856 (4)	0.854 (7)	**0.877 (8)**	0.838 (5)
sonar	**0.735 (95)**	**0.740 (91)**	0.706 (121)	0.655 (189)	**0.721 (113)**
spambase	0.876 (27)	0.756 (61)	0.887 (42)	0.881 (58)	**0.903 (18)**
splice	0.785 (49)	**0.799 (46)**	0.785 (55)	0.771 (67)	**0.801 (45)**
w8a	0.297 (80)	0.284 (96)	0.735 (35)	**0.742 (29)**	**0.745 (26)**

(F_1-measure is shown)

model: $f_\theta(x) = \theta^\top x$

surrogate loss: $\phi(m) = \max\{\log(1+e^{-m}), \log(1+e^{-\frac{m}{3}})\}$

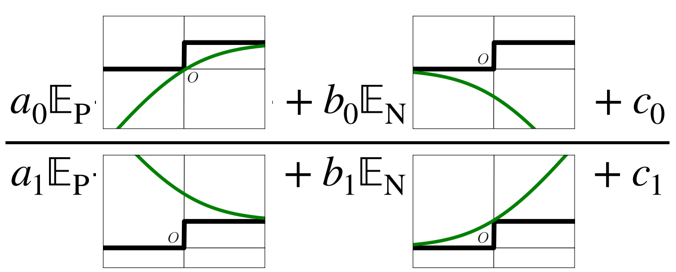
Loss for Complicated Metrics

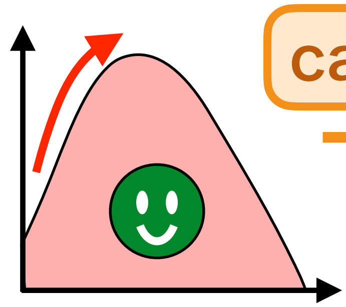
Linear-fractional metrics

contains F-measure, Jaccard
often used with imbalanced data

$$U(f) = \frac{a_0\mathrm{TP} + b_0\mathrm{FP} + c_0}{a_1\mathrm{TP} + b_1\mathrm{FP} + c_1}$$

surrogate utility

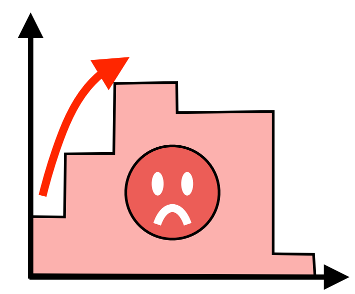




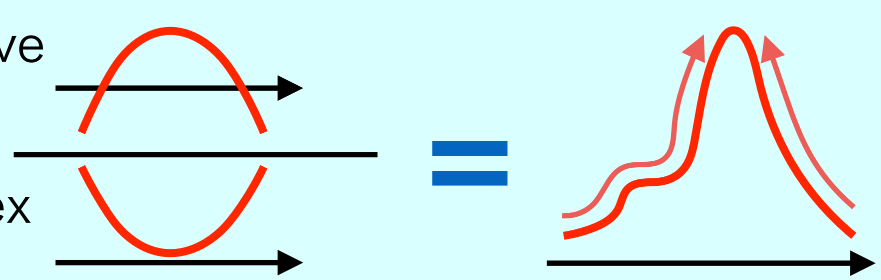
calibrated

target utility

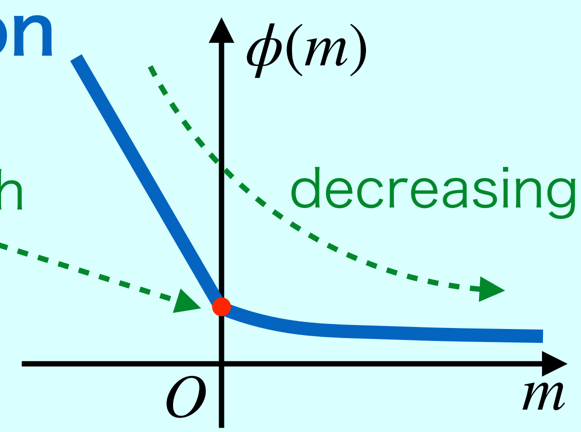
$$U(f) = \frac{a_0\mathrm{TP} + b_0\mathrm{FP} + c_0}{a_1\mathrm{TP} + b_1\mathrm{FP} + c_1}$$



①tractability (quasi-concave)



②calibration



Provides guideline of designing loss for complicated metrics!

When adversary presents

H. Bao, C. Scott, and M. Sugiyama.
Calibrated Surrogate Losses for Adversarially Robust Classification.
In *COLT*, 2020.

Adversarial Attacks

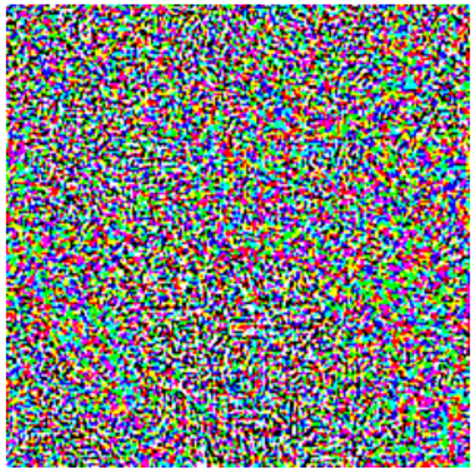
[Goodfellow+ 2015]

Adding inperceptible small noise can fool classifiers!

original data

perturbed data

$+\ .007 \times$



$=$

$\boldsymbol{x}$

"panda"
57.7% confidence

$\mathrm{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$

"nematode"
8.2% confidence

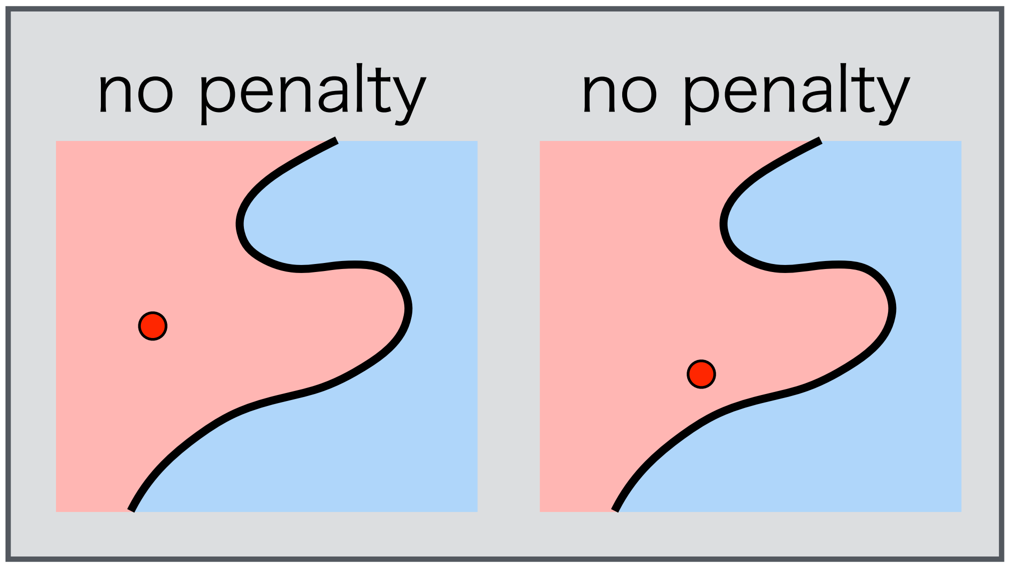
$\boldsymbol{x} + \epsilon \mathrm{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$

"gibbon"
99.3 % confidence

Goodfellow, I. J., Shlens, J., & Szegedy, C. (2015). Explaining and harnessing adversarial examples. In *ICLR*, 2015.

Penalize Vulnerable Prediction

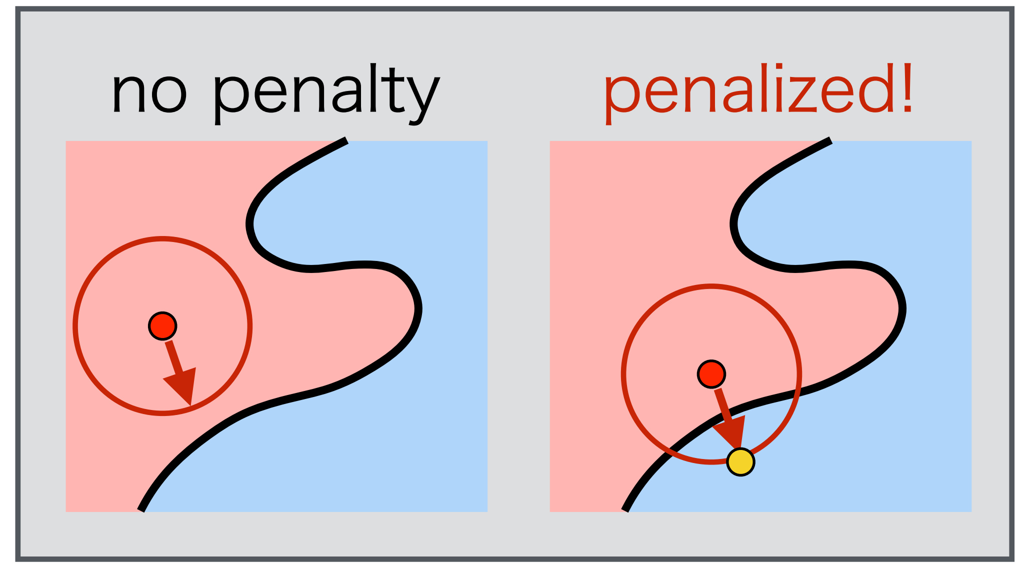
Usual Classification



usual 0-1 loss

$$\ell_{01}(x, y, f) = \begin{cases} 1 \text{ if } yf(x) \leq 0 \\ 0 \text{ otherwise} \end{cases}$$

Robust Classification



robust 0-1 loss

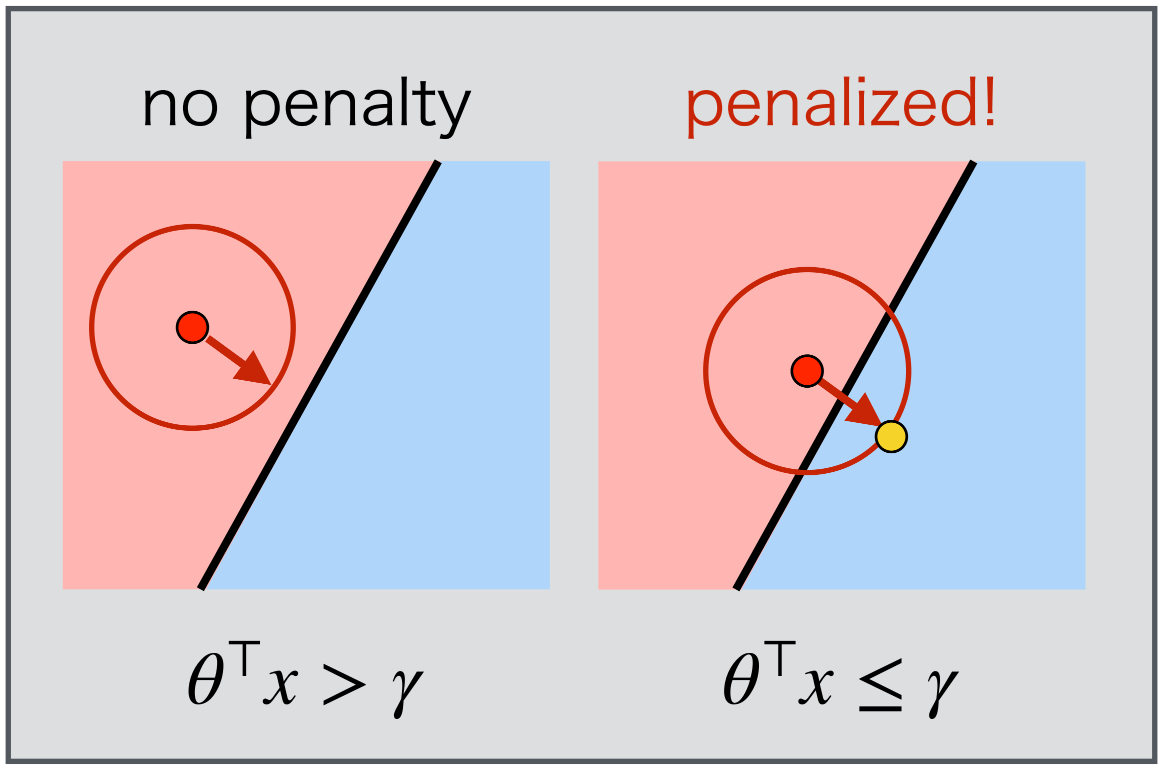
$$\ell_{\gamma}(x, y, f) = \begin{cases} 1 & \text{if } \exists \Delta \in \mathbb{B}_2(\gamma) \,.\, yf(x + \Delta) \leq 0 \\ 0 & \text{otherwise} \end{cases}$$

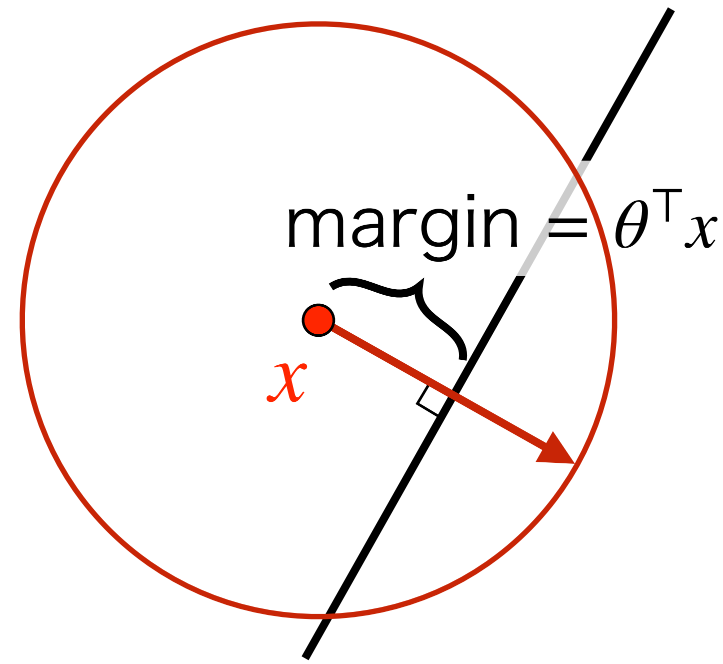
prediction too close to boundary should be penalized

$\mathbb{B}_2(\gamma) = \{x \in \mathbb{R}^d \mid \|x\|_2 \leq \gamma\}$: γ-ball

In Case of Linear Predictors

linear predictors $\mathscr{F}_{\mathrm{lin}} = \{x \mapsto \theta^\top x \mid \|\theta\|_2 = 1\}$





robust 0-1 loss

$$\ell_\gamma(x, y, f) = \begin{cases} 1 & \text{if } \exists \Delta \in \mathbb{B}_2(\gamma)\,.\, yf(x+\Delta) \leq 0 \\ 0 & \text{otherwise} \end{cases} \quad = \quad \mathbf{1}\{yf(x) \leq \gamma\} := \phi_\gamma(yf(x))$$

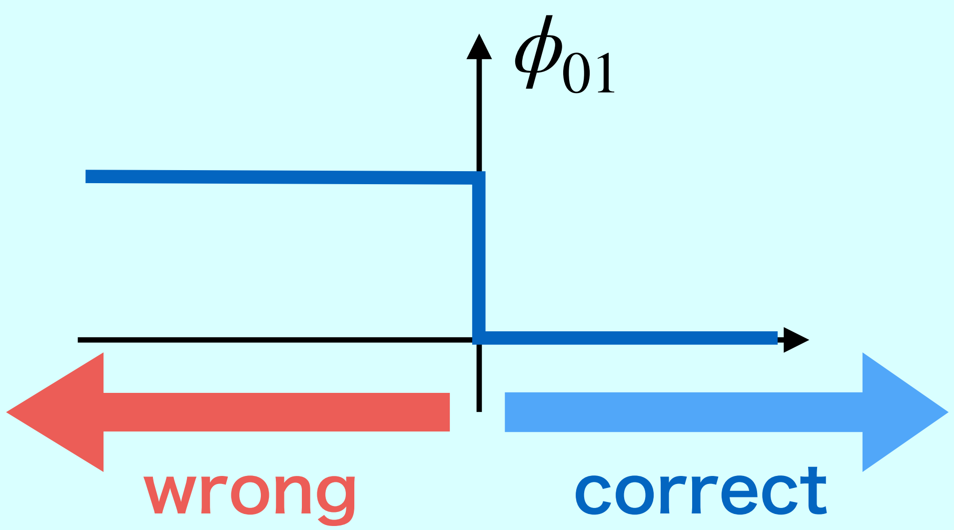
Formulation of Classification

Usual Classification

minimize 0-1 risk

$$R_{\phi_{01}}(f) = \mathbb{E}\left[\phi_{01}(Yf(X))\right]$$

0-1 loss $\phi_{01}(\alpha) = \mathbf{1}\{\alpha \le 0\}$



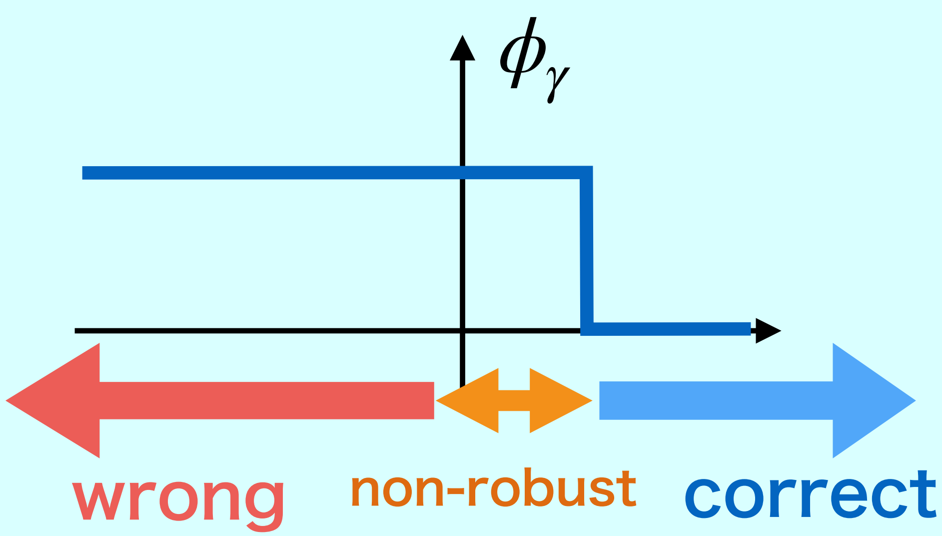
Robust Classification

minimize γ-robust 0-1 risk

$$R_{\phi_\gamma}(f) = \mathbb{E}\left[\phi_\gamma(Yf(X))\right]$$

(restricted to linear predictors)

robust 0-1 loss $\phi_\gamma(\alpha) = \mathbf{1}\{\alpha \le \gamma\}$

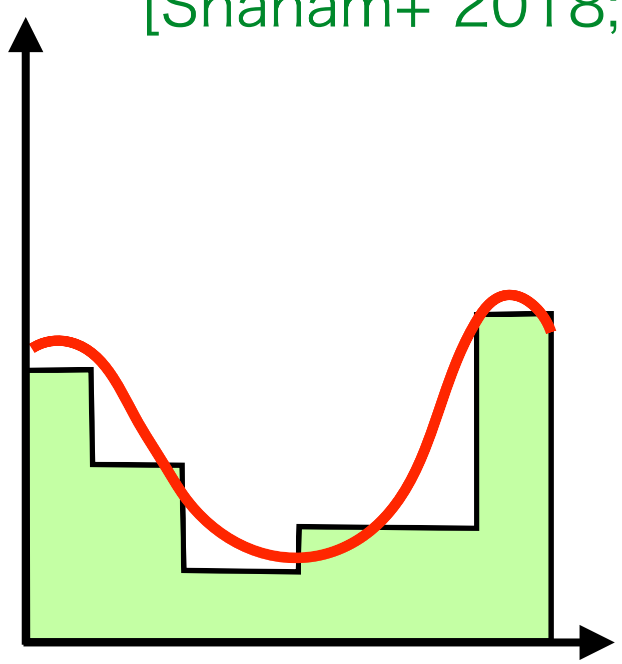


Existing Approaches

Direct optimization of robust risk $R_{\phi_\gamma}(f)$ is intractable

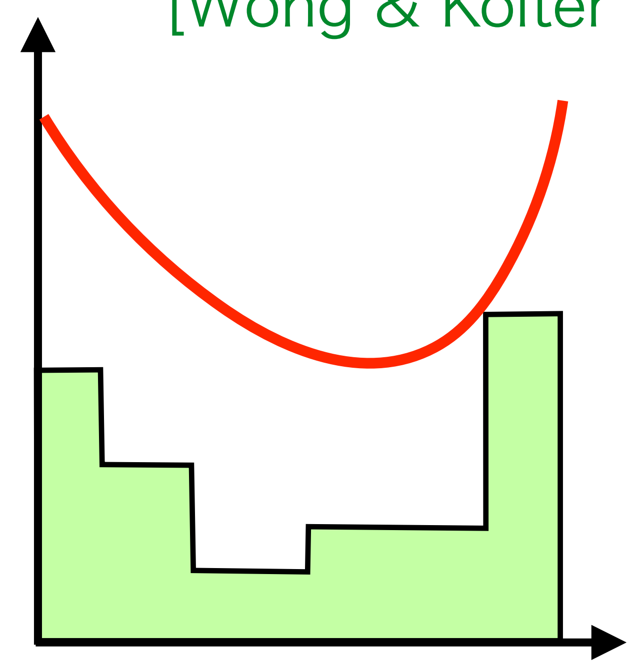
Taylor approximation

[Shaham+ 2018; etc.]



Convex upper bound

[Wong & Kolter 2018; etc.]



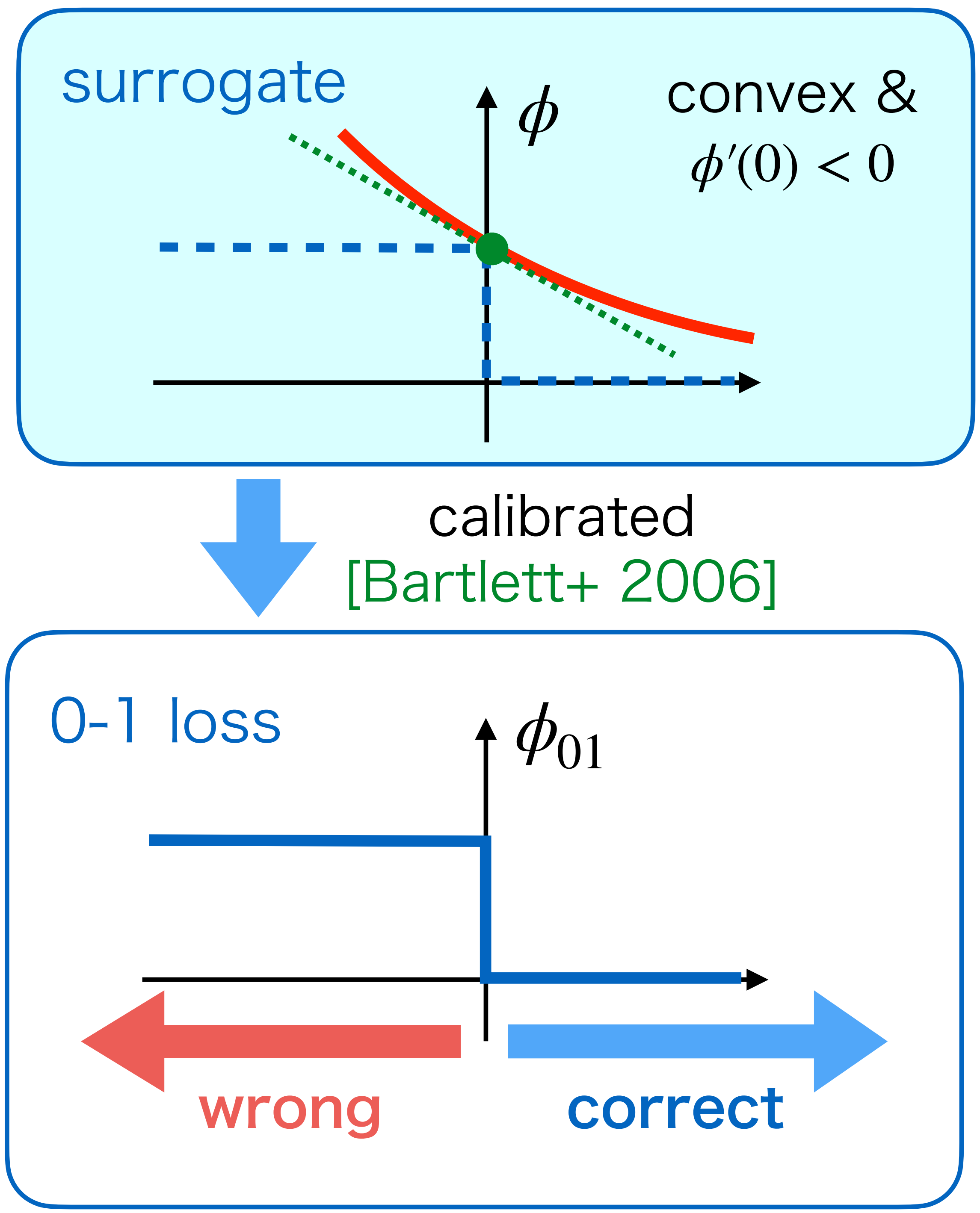
Both do not necessarily lead to true minimizer!

Shaham, U., Yamada, Y., & Negahban, S. (2018).
Understanding adversarial training: Increasing local stability of supervised models through robust optimization. *Neurocomputing*, 195-204.

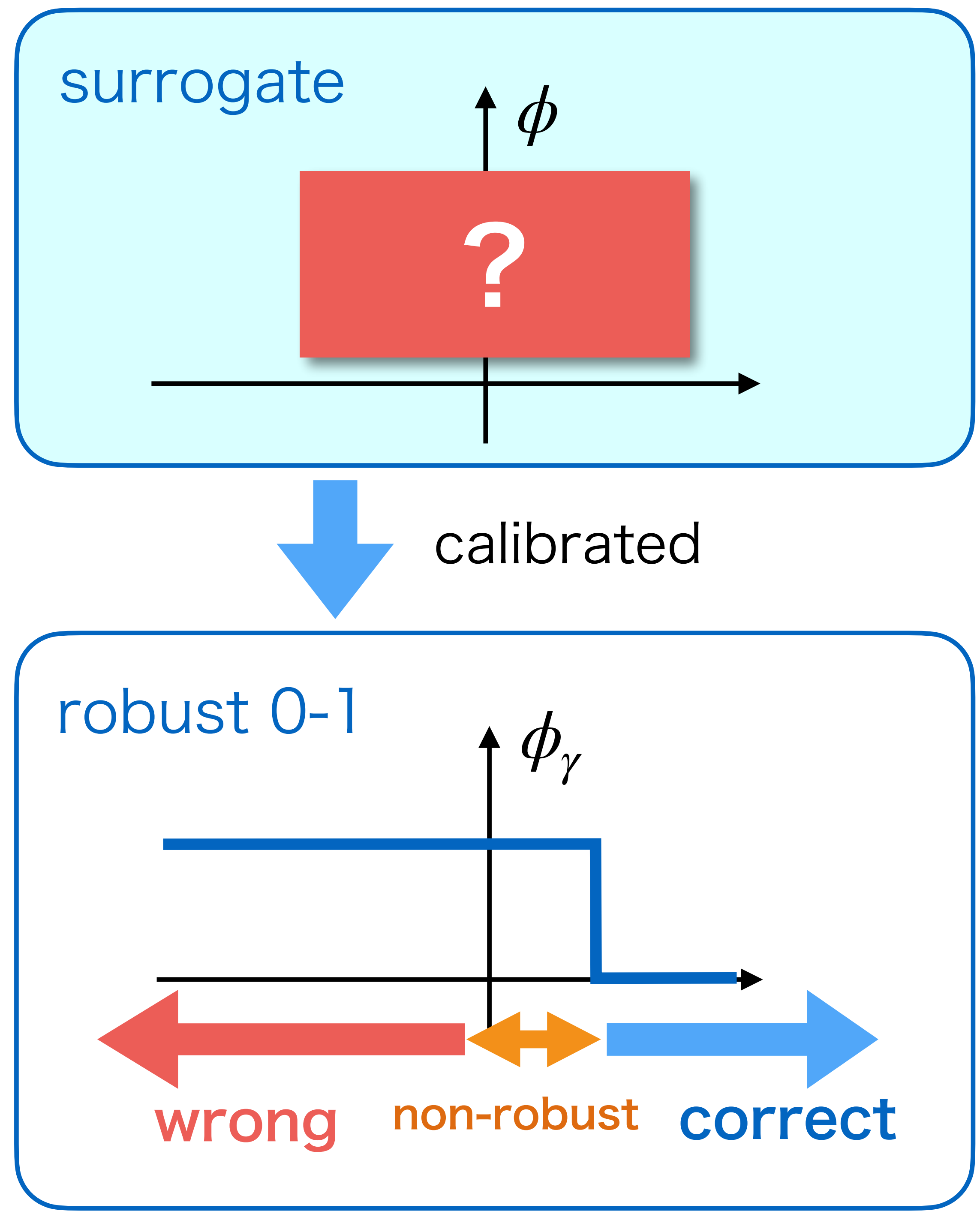
Wong, E., & Kolter, Z. (2018,). Provable Defenses against Adversarial Examples via the Convex Outer Adversarial Polytope.
In *International Conference on Machine Learning* (pp. 5286-5295).

What surrogate is calibrated?

Usual Classification



Robust Classification

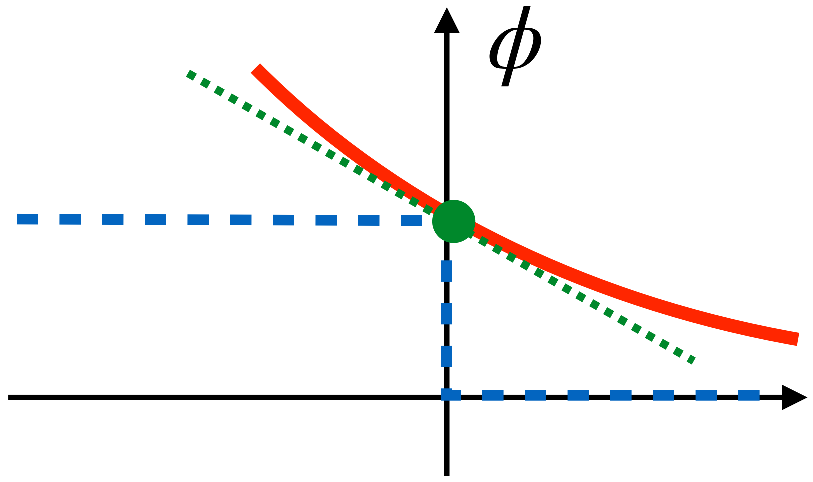


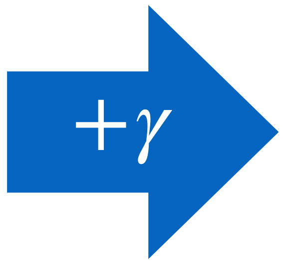
P. L. Bartlett, M. I. Jordan, & J. D. McAuliffe. (2006).
Convexity, classification, and risk bounds. *Journal of the American Statistical Association*, 101(473), 138-156.

Isn't it a piece of cake?

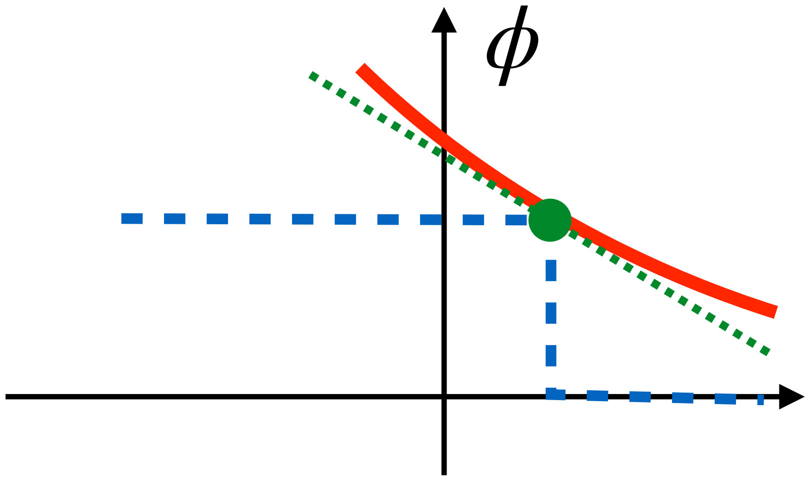
Theorem. If surrogate ϕ is convex, it is ϕ_{01}-calibrated iff
- differentiable at 0
- $\phi'(0) < 0$

Usual 0-1 loss





Robust 0-1 loss



If $\phi'(\gamma) < 0$, then calibrated to robust 0-1 loss?

No convex calibrated surrogate

Theorem. Any convex surrogate is not ϕ_γ-calibrated.

(under linear predictors)

Proof Sketch: find distribution such that $\delta(\varepsilon) = 0$

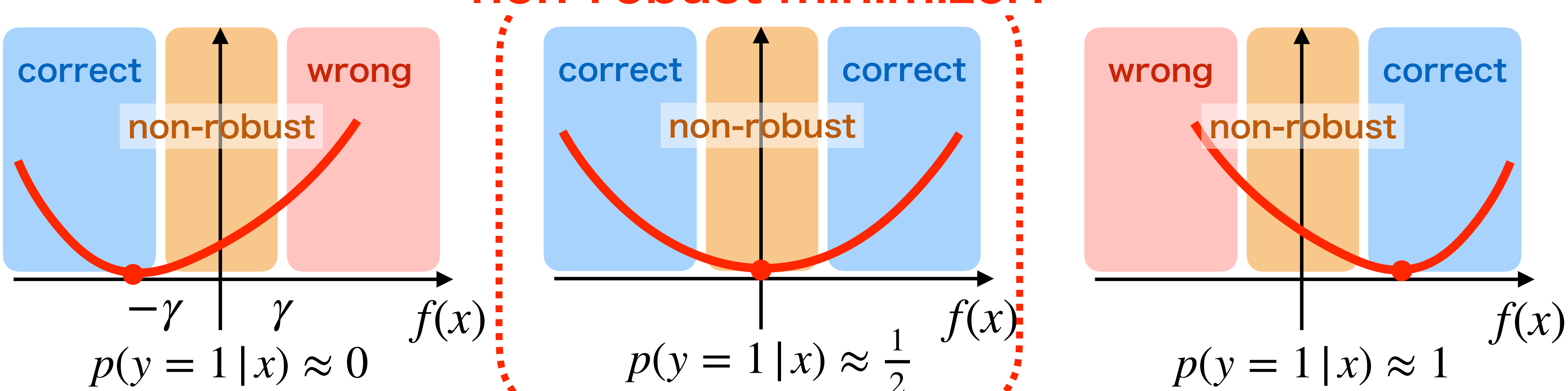
calibration function

convex in f

interpretation:
f is non-robust ($|f(x)| < \gamma$)

$$\delta(\varepsilon) = \inf_f R_\phi(f) - R_\phi^* \quad \text{s.t.} \quad R_{\phi_\gamma}(f) - R_{\phi_\gamma}^* \geq \varepsilon$$

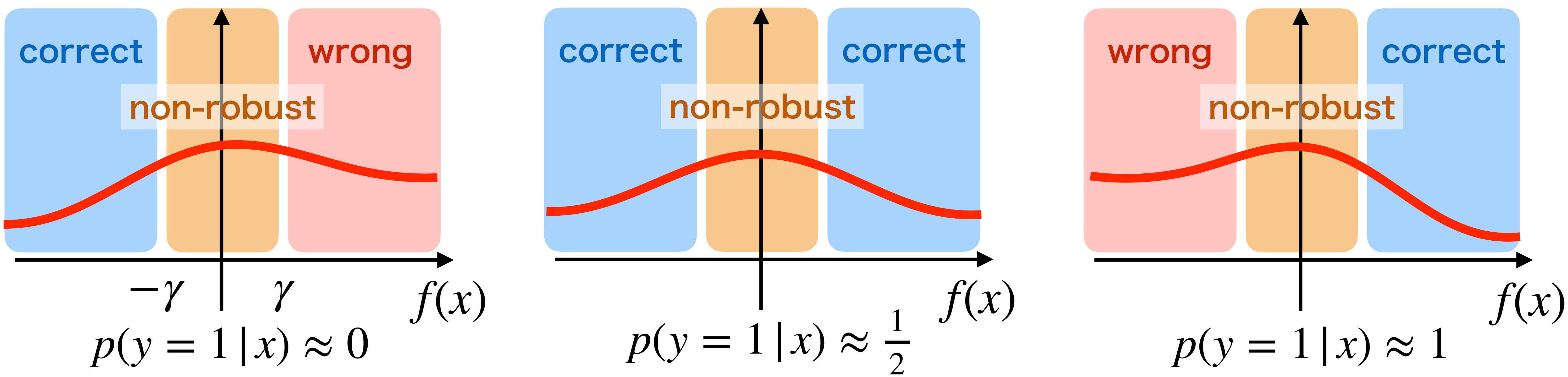
non-robust minimizer!



surrogate **conditional** risk is plotted

How to find calibrated surrogate?

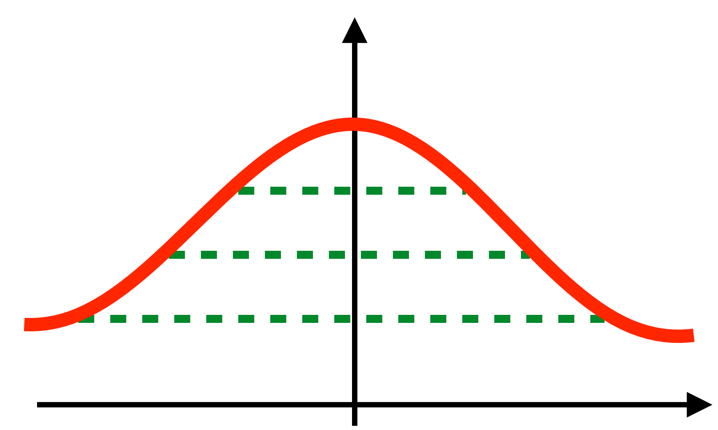
Idea. To make conditional risk not minimized in **non-robust area**



surrogate conditional risk is plotted

consider a surrogate ϕ such that

conditional risk is **quasiconcave**

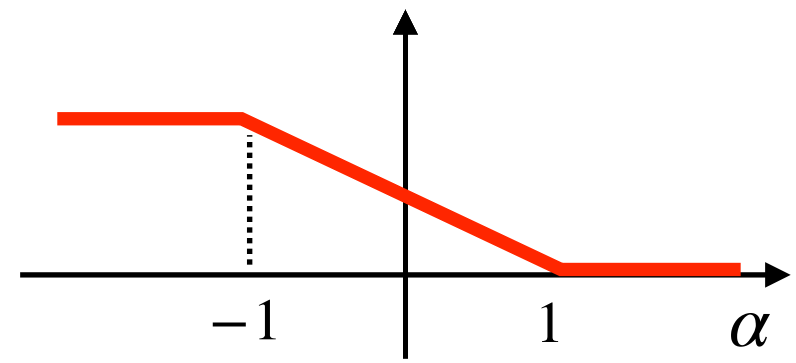


all superlevels are convex

Example: Shifted Ramp Loss

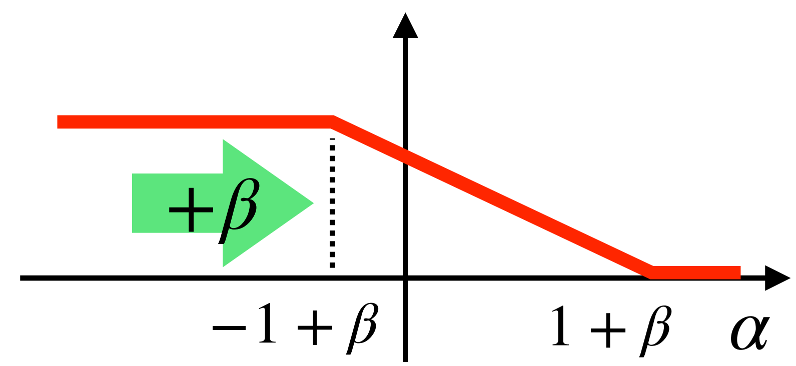
Ramp loss

$$\phi(\alpha) = \mathrm{clip}_{[0,1]}\left(\frac{1-\alpha}{2}\right)$$

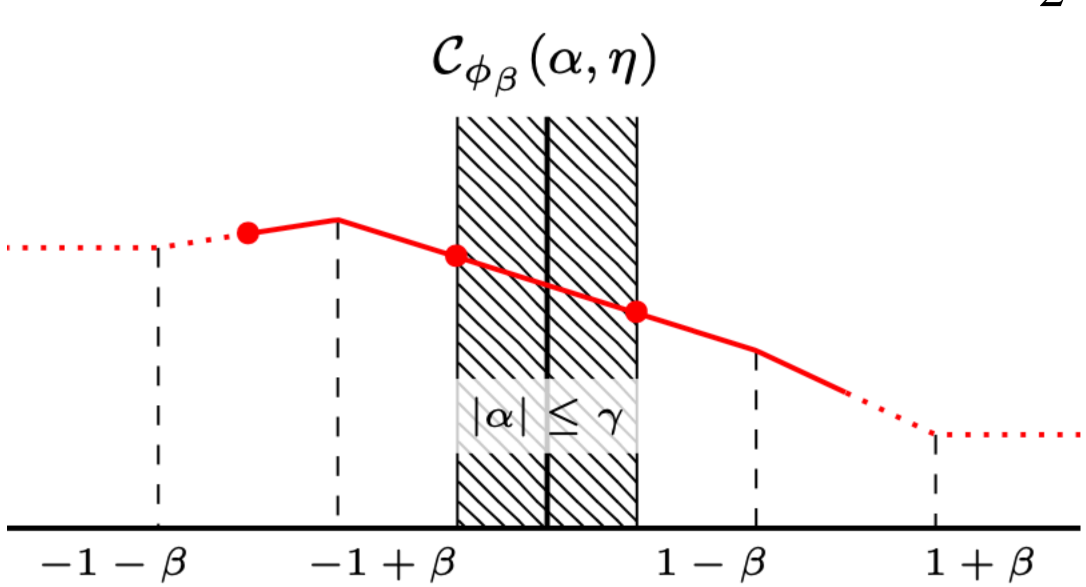


Shifted ramp loss

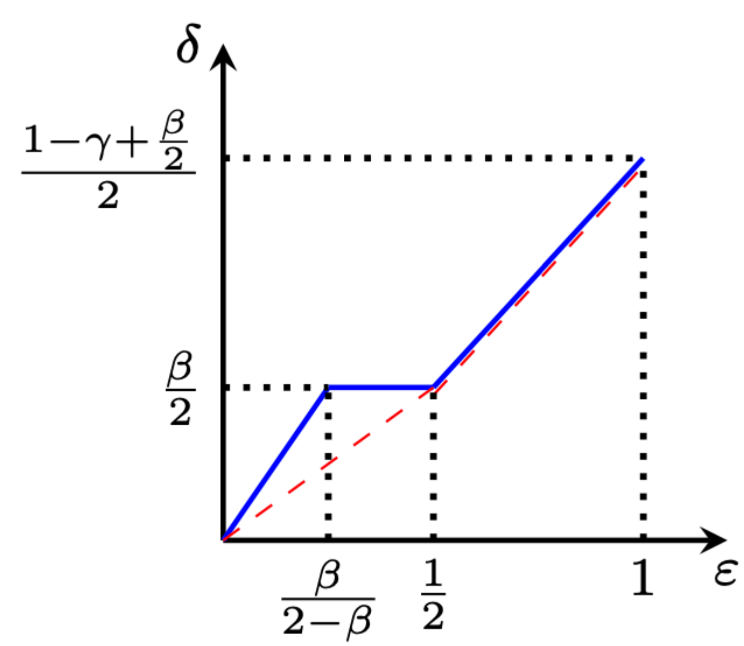
$$\phi_\beta(\alpha) = \mathrm{clip}_{[0,1]}\left(\frac{1-\alpha+\beta}{2}\right)$$



conditional risk $(p(y=1\,|\,x) > \frac{1}{2})$



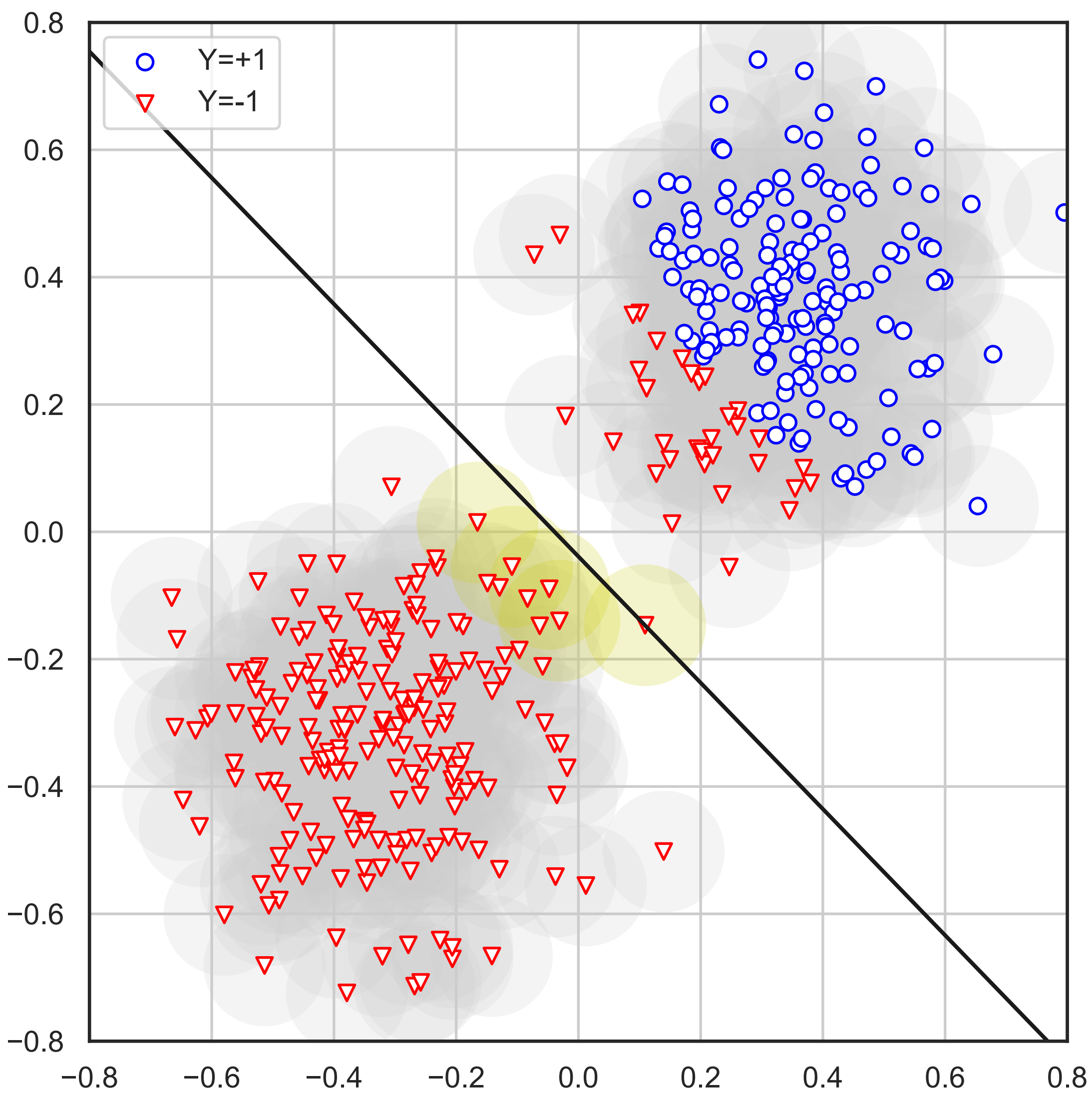
calibration function



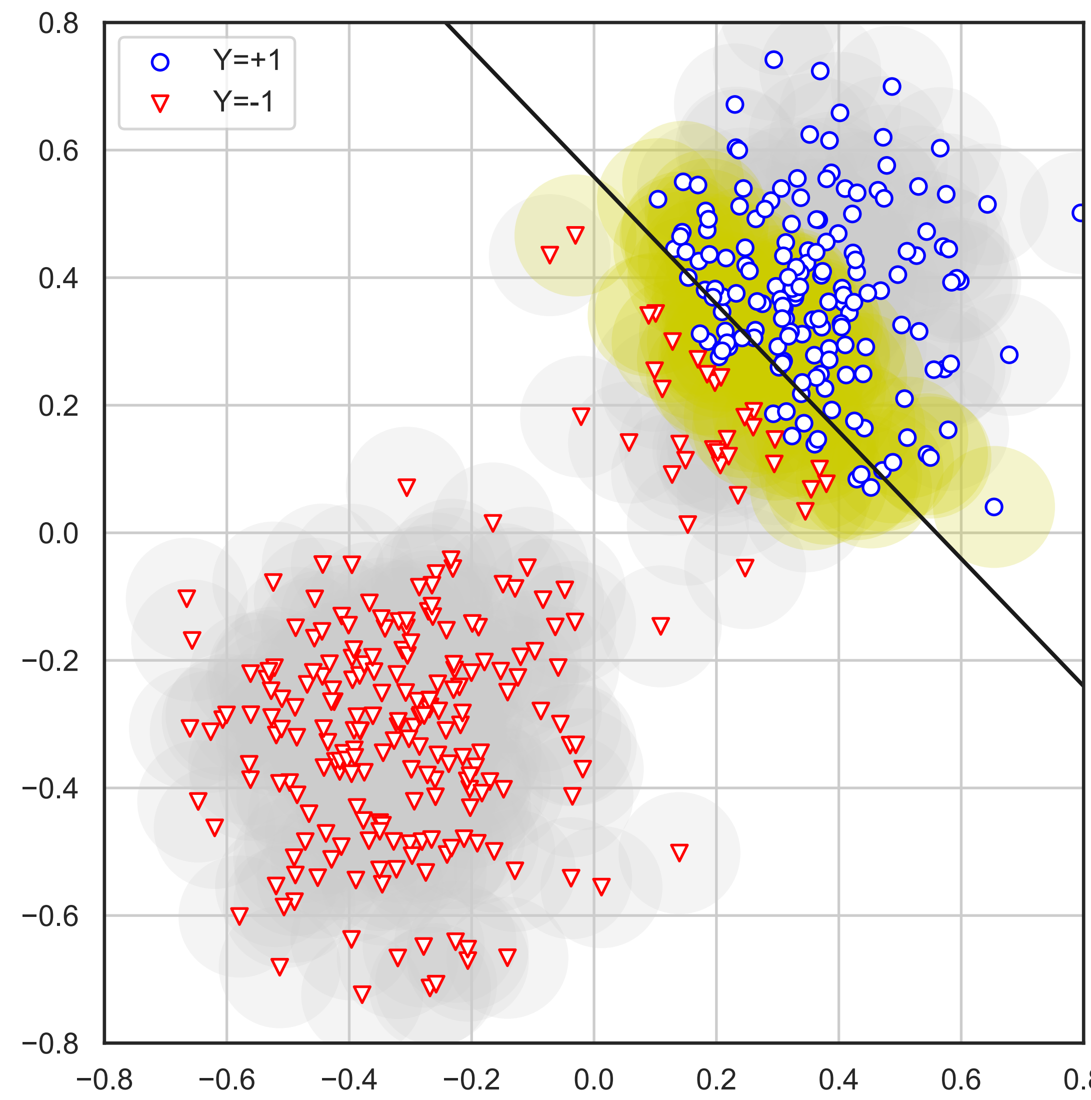
assume $0 < \beta < 1-\gamma$

Simulation

Ramp loss



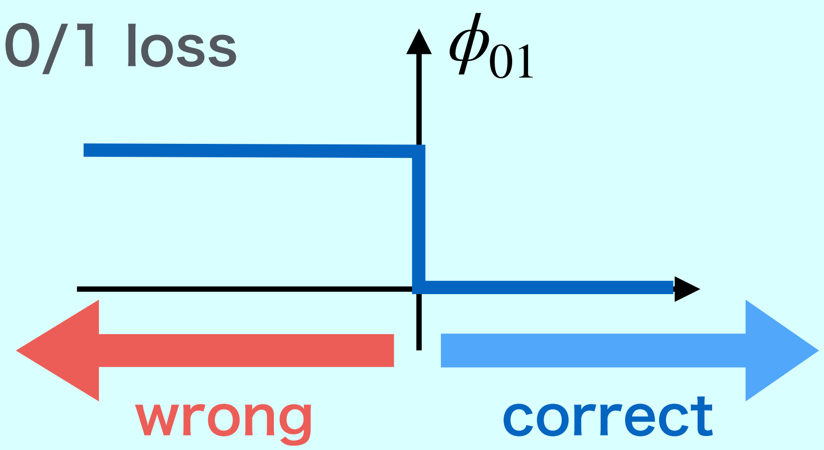
Hinge loss

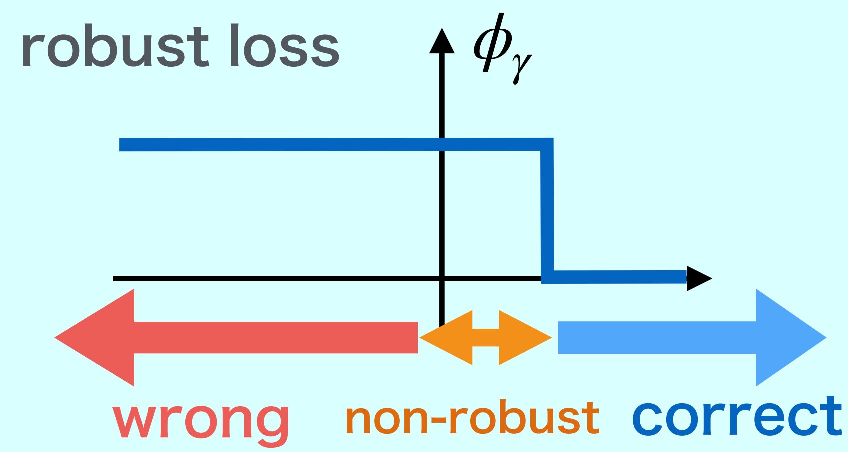


each ball is γ-ball / yellow balls are non-robust data points

Loss for Robust Learning

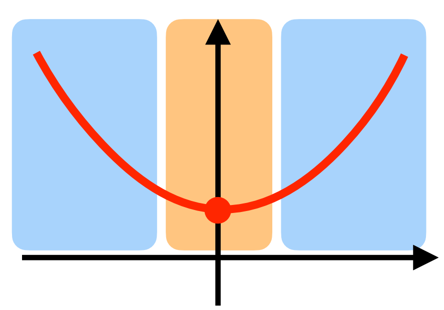
“Embed” robustness into loss function



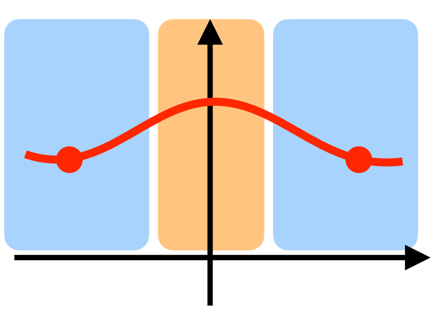


loss function can not only accommodate classification performance but also robustness

Inability of convex loss



convex loss is minimized in non-robust area

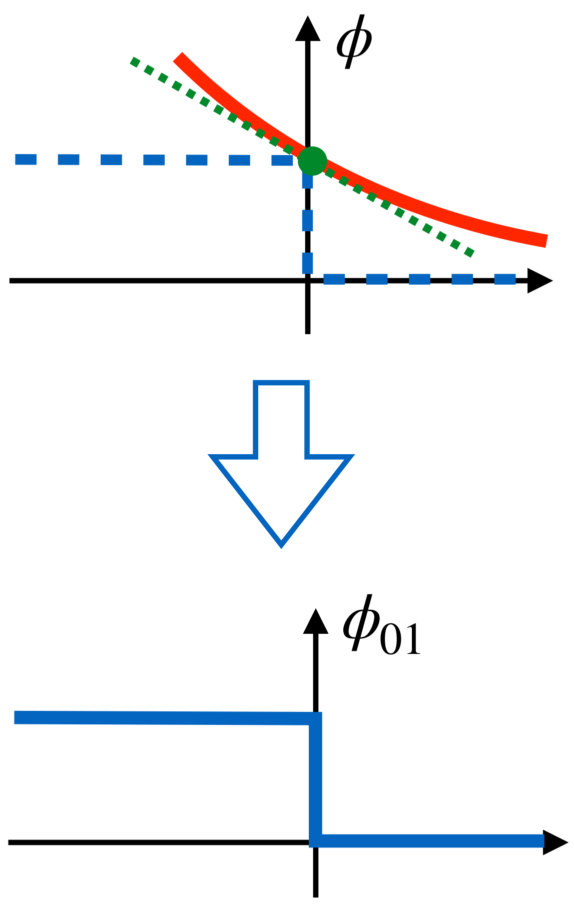


robust objective

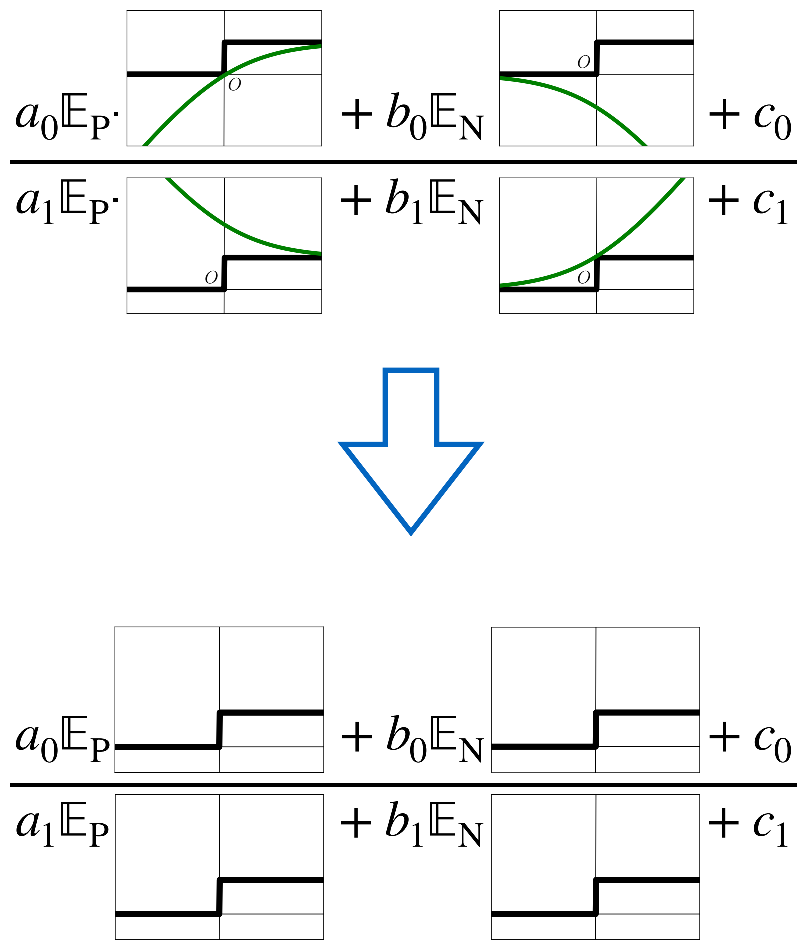
Calibration theory helps to reveal classifiers’ property!

Summary

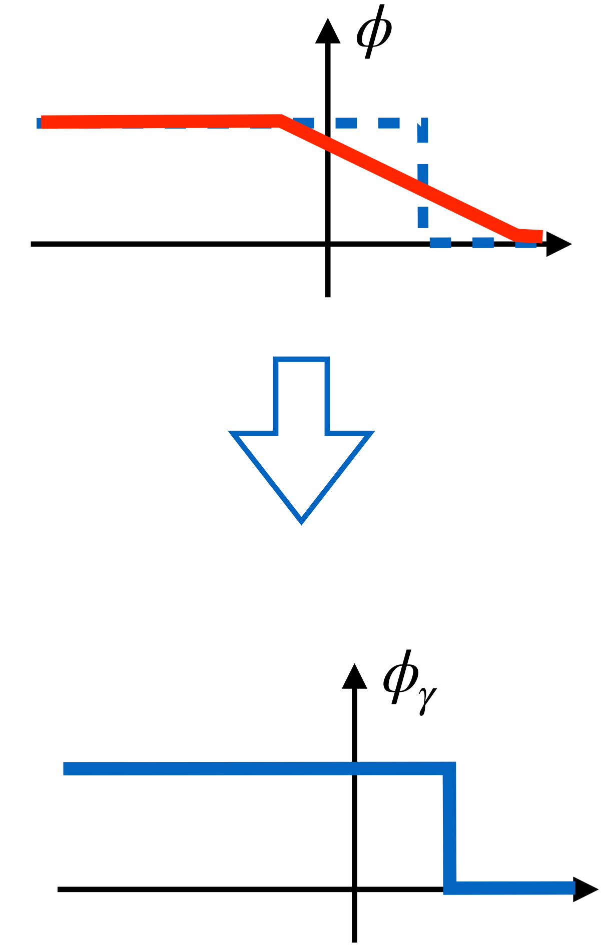
Binary Classification



Linear-fractional Metrics



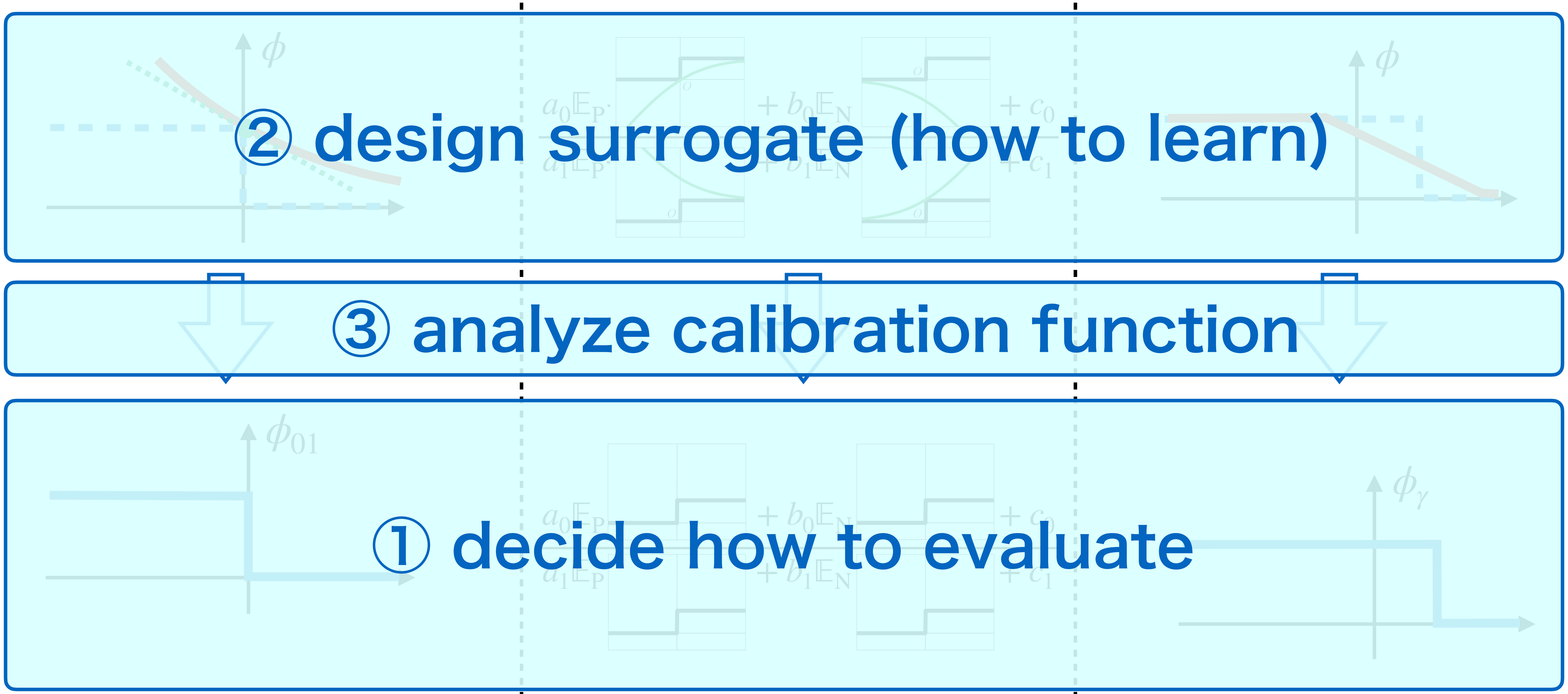
Adversarial Robustness



- Introduce calibration analysis
- Show applicability to analyze robustness

Summary

Binary Classification | **Linear-fractional Metrics** | **Adversarial Robustness**



- Introduce calibration analysis
- Show applicability to analyze robustness

More Reads

classification

- binary [Lin04] [Zha04a] [BJM06] [WL07]
- multi-class [Zha04b] [TB07] [LS13] [PS16] [RA16]
- cost-sensitive [Sco12]
- imbalance [BS20]

ranking

- AUC [DKH12] [GZ15]
- top-k [Blo19] [YK20]
- preference graph [DMJ10]
- NDCG [RTY11] [Blo19]
- precision@k [RAT13]
- pAp@k [HVK+20]

structured prediction

- abstain [RA16] [NCH+19]
- multi label [GZ11] [ZRA20]
- partial label [CGS11] [CRB20]
- ordinal [RA16] [PBG18]
- Hamming [OBL17] [NBR20]

robustness

- label noise [RW10]
- adversarial [BSS20]

Any new problems?