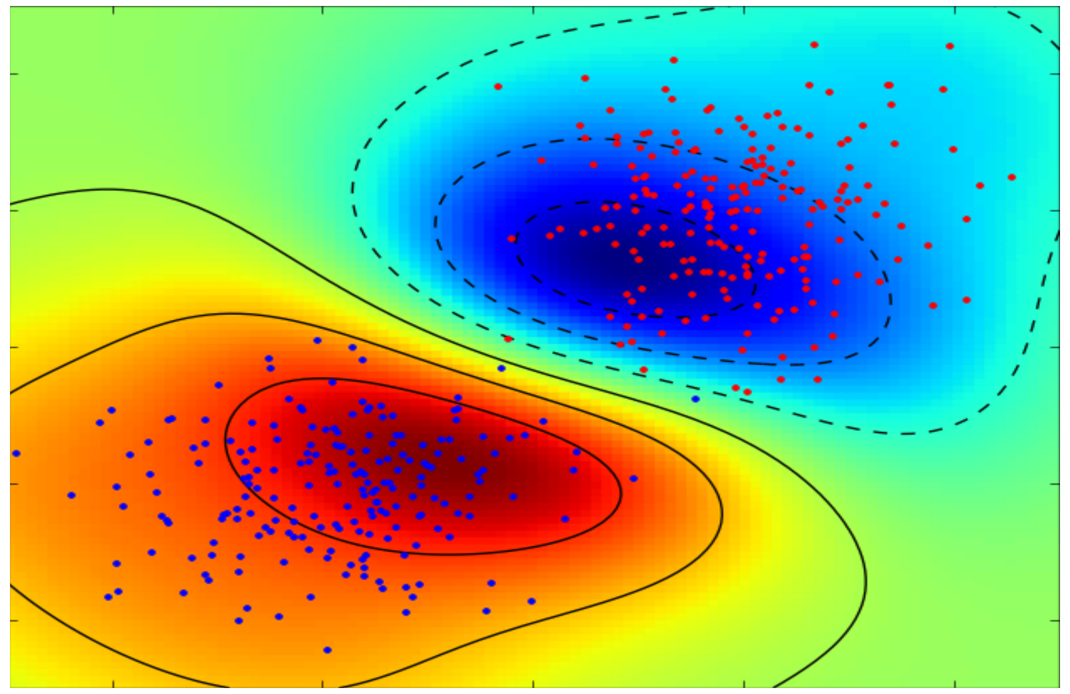
Regularization via Optimal Transport

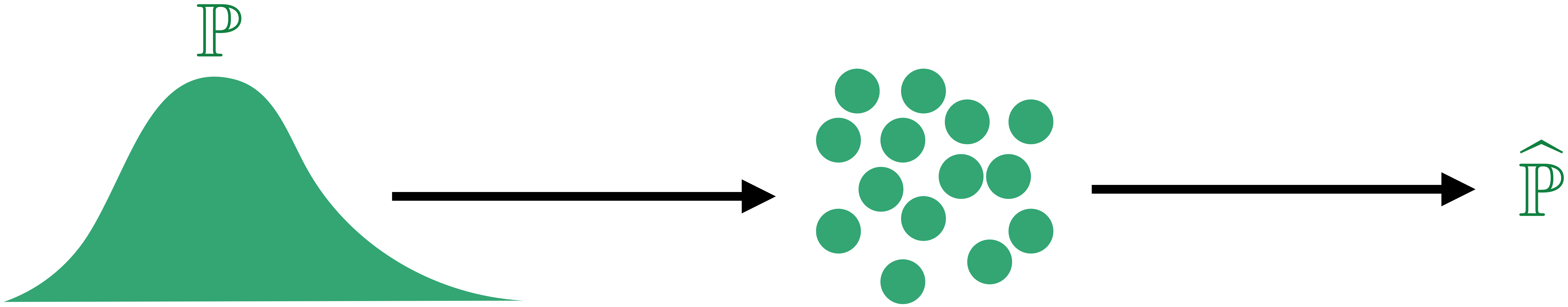
Soroosh Shafieezadeh Abadeh, Tepper School of Business, CMU

Stochastic Programming

$$\inf_{\theta \in \Theta} \mathbb{E}_{\mathbb{P}} \left[\ell(\theta, \xi) \right]$$

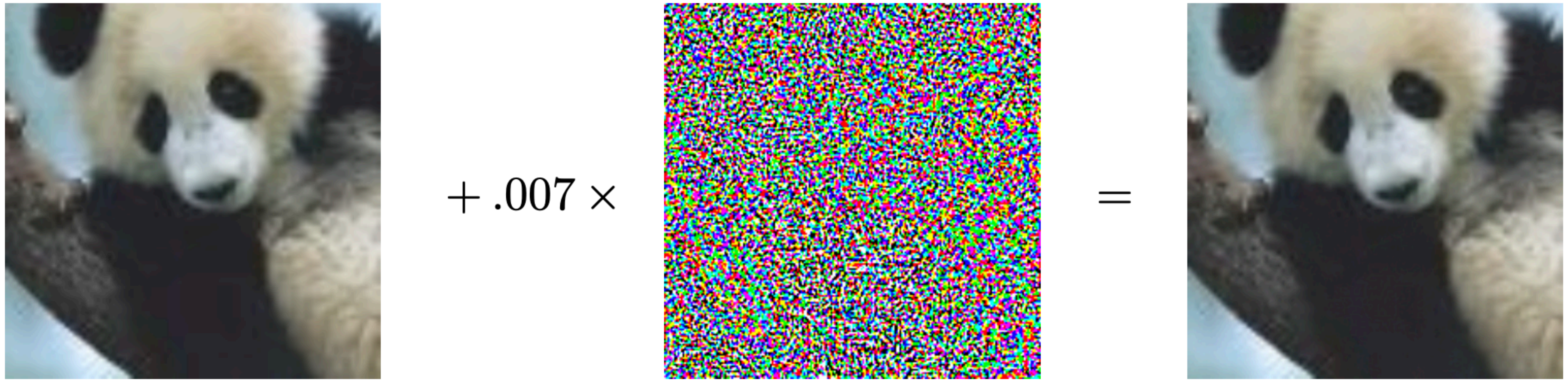


Failure Examples: Overfitting



$$\inf_{\theta \in \Theta} \; \mathbb{E}_{\widehat{\mathbb{P}}}\left[\ell(\theta, \xi)\right]$$

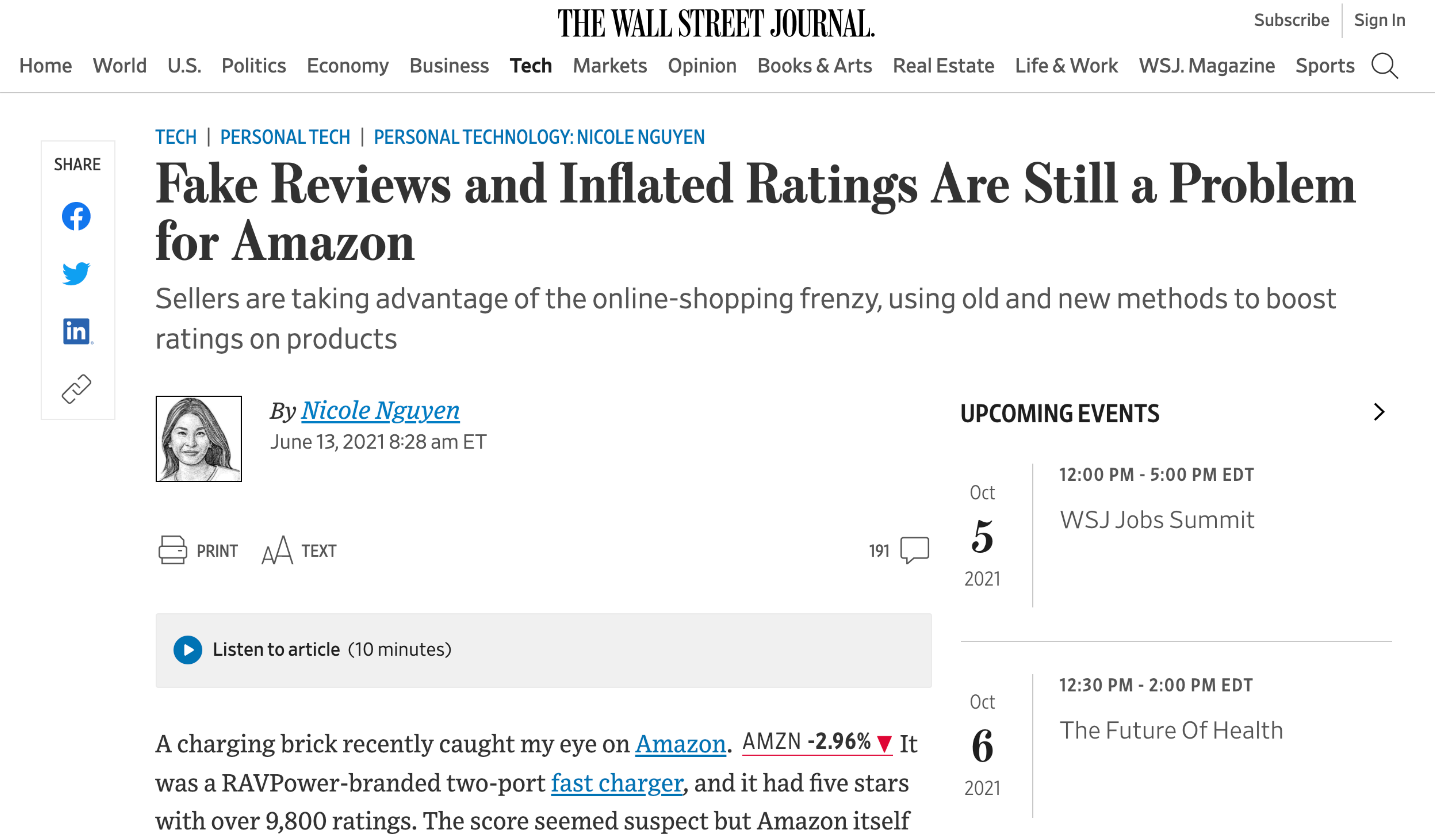
Failure Examples: Adversarial Attack [GSS15]



Panda
57.7% Confidence

Gibbon
99.3% Confidence

Failure Examples: Fake Data



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Fake Reviews and Inflated Ratings Are Still a Problem for Amazon

Sellers are taking advantage of the online-shopping frenzy, using old and new methods to boost ratings on products

By Nicole Nguyen
June 13, 2021 8:28 am ET

PRINT TEXT 191

Listen to article (10 minutes)

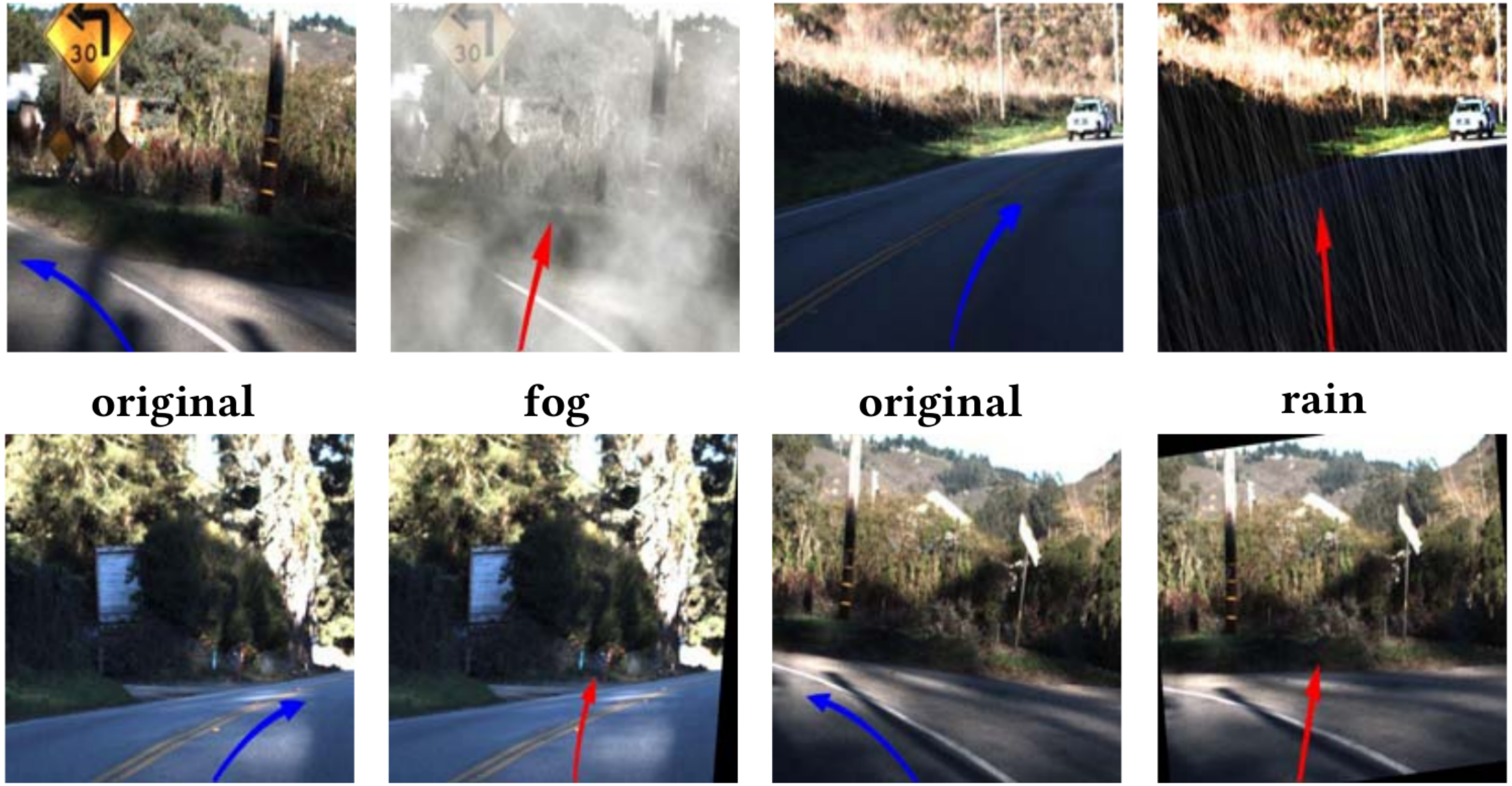
A charging brick recently caught my eye on Amazon. AMZN **-2.96%** ▼ It was a RAVPower-branded two-port fast charger, and it had five stars with over 9,800 ratings. The score seemed suspect but Amazon itself

UPCOMING EVENTS

Oct 5 2021
12:00 PM - 5:00 PM EDT
WSJ Jobs Summit

Oct 6 2021
12:30 PM - 2:00 PM EDT
The Future Of Health

Failure Examples: Domain Change [TPJR18]



original

fog

original

rain

original

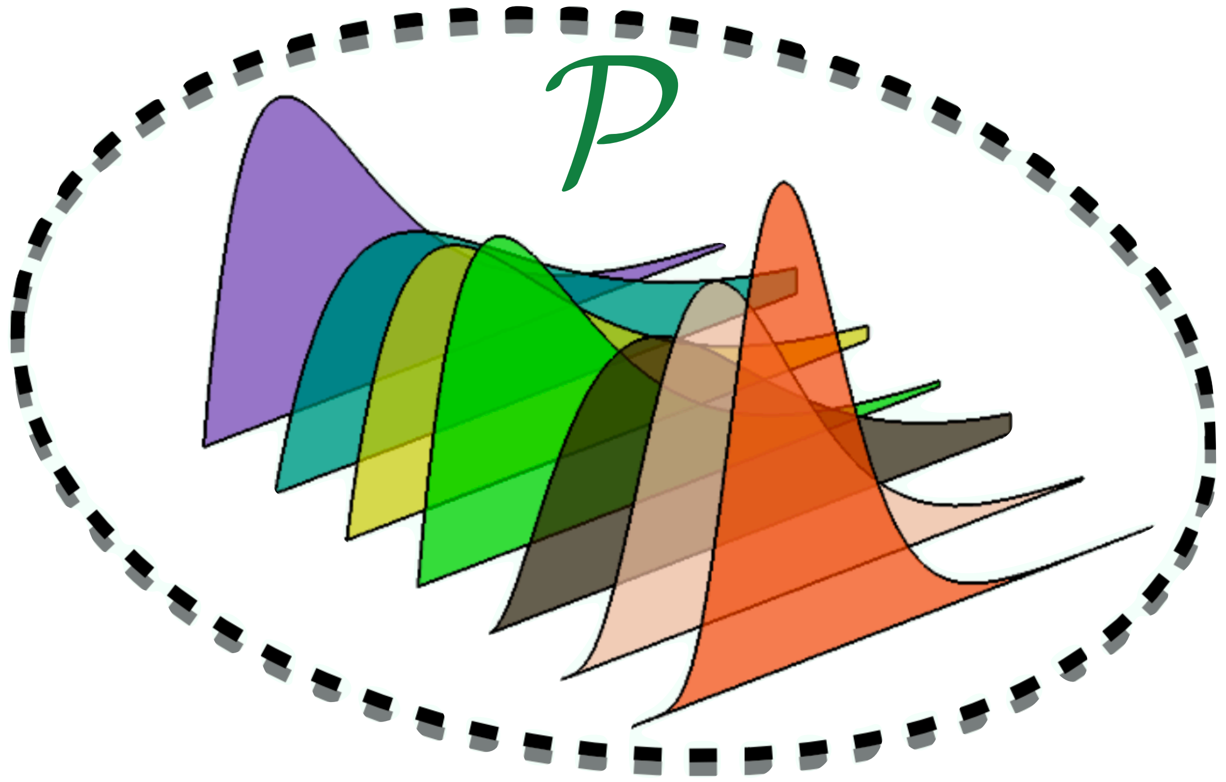
shear(0.1)

original

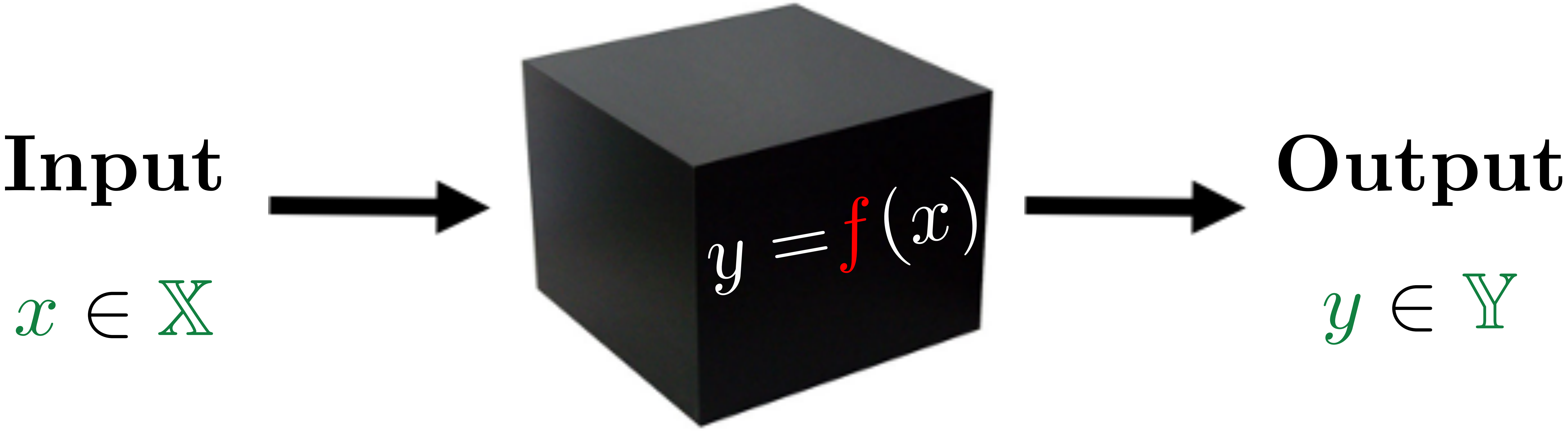
rotation(6 degree)

Distributionally Robust Optimization

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\ell(\theta, \xi) \right]$$



Supervised Learning



Input

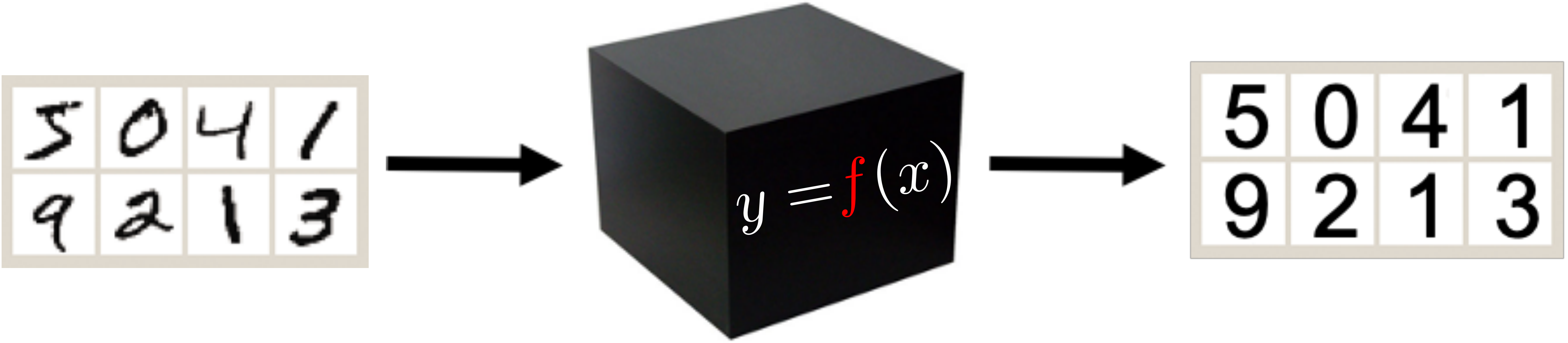
$x \in \mathbb{X}$

$y = f(x)$

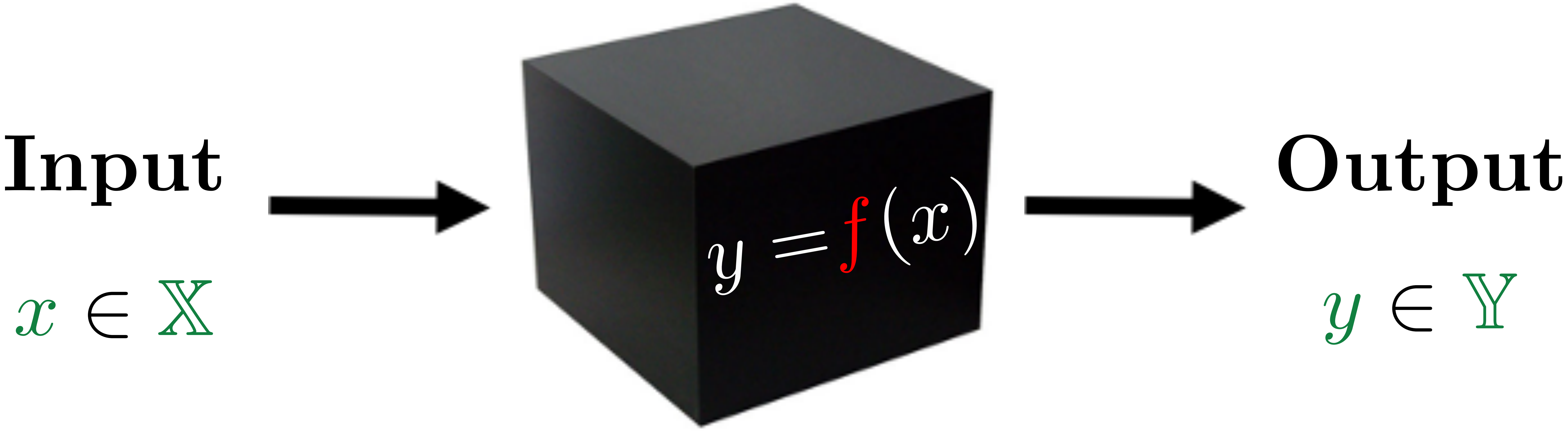
Output

$y \in \mathbb{Y}$

Supervised Learning



Supervised Learning



Input

$x \in \mathbb{X}$

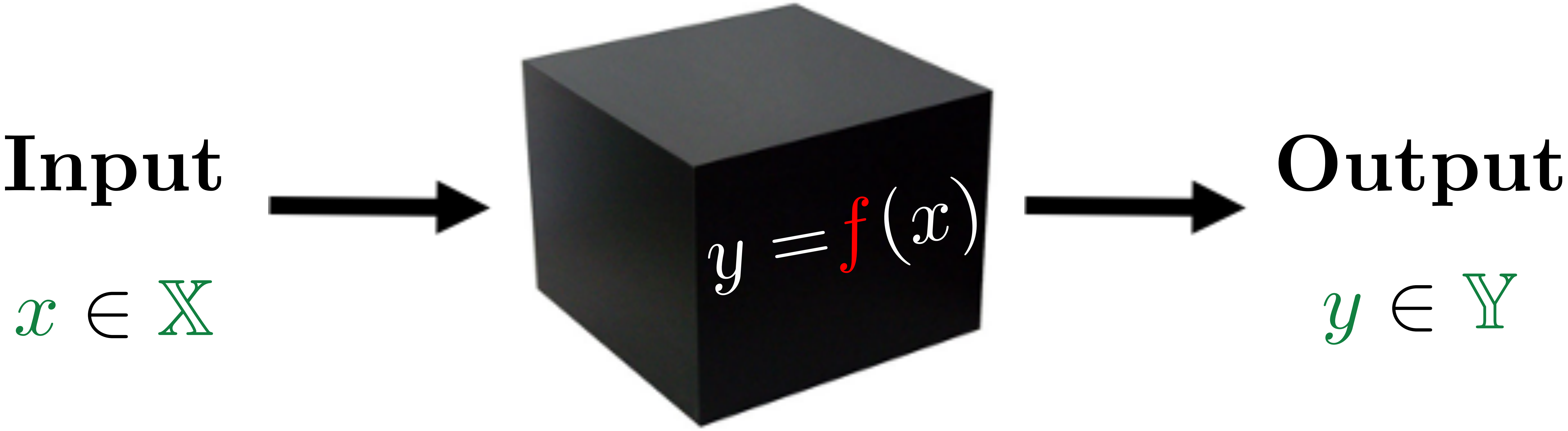
$y = {\color{red} f}(x)$

Output

$y \in \mathbb{Y}$

Training data: $\widehat{\Xi}_N = (\widehat{x}_1, \widehat{y}_1), \ldots (\widehat{x}_N, \widehat{y}_N)$

Supervised Learning



Input

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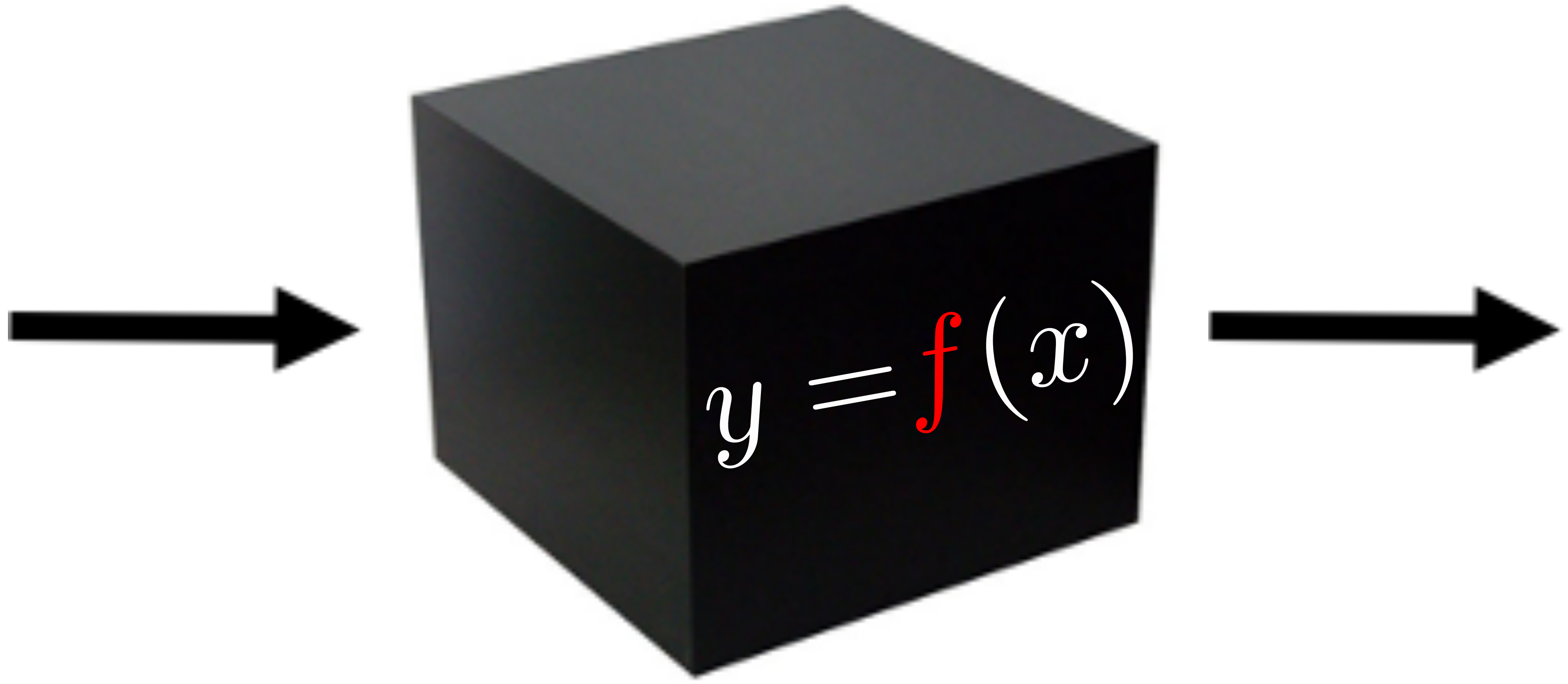
Output

$y \in \mathbb{Y}$

Training data: $\widehat{\Xi}_N = (\widehat{x}_1, \widehat{y}_1), \ldots (\widehat{x}_N, \widehat{y}_N)$

Hypothesis space: $\mathbb{H} \subseteq \{h \in \mathbb{R}^{\mathbb{X}}\}$

Supervised Learning



Input

$x \in \mathbb{X}$

$y = f(x)$

Output

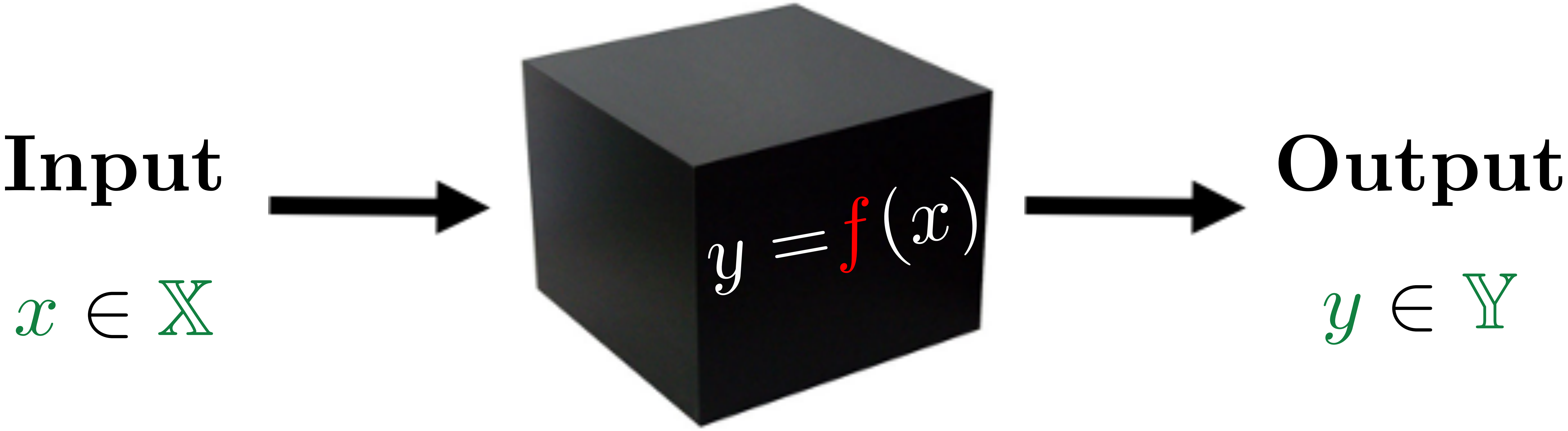
$y \in \mathbb{Y}$

Training data: $\widehat{\Xi}_N = (\widehat{x}_1, \widehat{y}_1), \ldots (\widehat{x}_N, \widehat{y}_N)$

Hypothesis space: $\mathbb{H} \subseteq \{h \in \mathbb{R}^{\mathbb{X}}\}$

Target function: $f(x) \approx h(x)$

Supervised Learning



Input

$x \in \mathbb{X}$

$y = f(x)$

Output

$y \in \mathbb{Y}$

Training data: $\widehat{\Xi}_N = (\widehat{x}_1, \widehat{y}_1), \ldots (\widehat{x}_N, \widehat{y}_N)$

Hypothesis space: $\mathbb{H} \subseteq \{h \in \mathbb{R}^{\mathbb{X}}\}$

Target function: $f(x) \approx h(x)$

Learning algorithm: $\inf_{h \in \mathbb{H}} \ \ell(h, \widehat{\Xi}_N)$

Regression Models

Target function: $f(x) = h(x)$

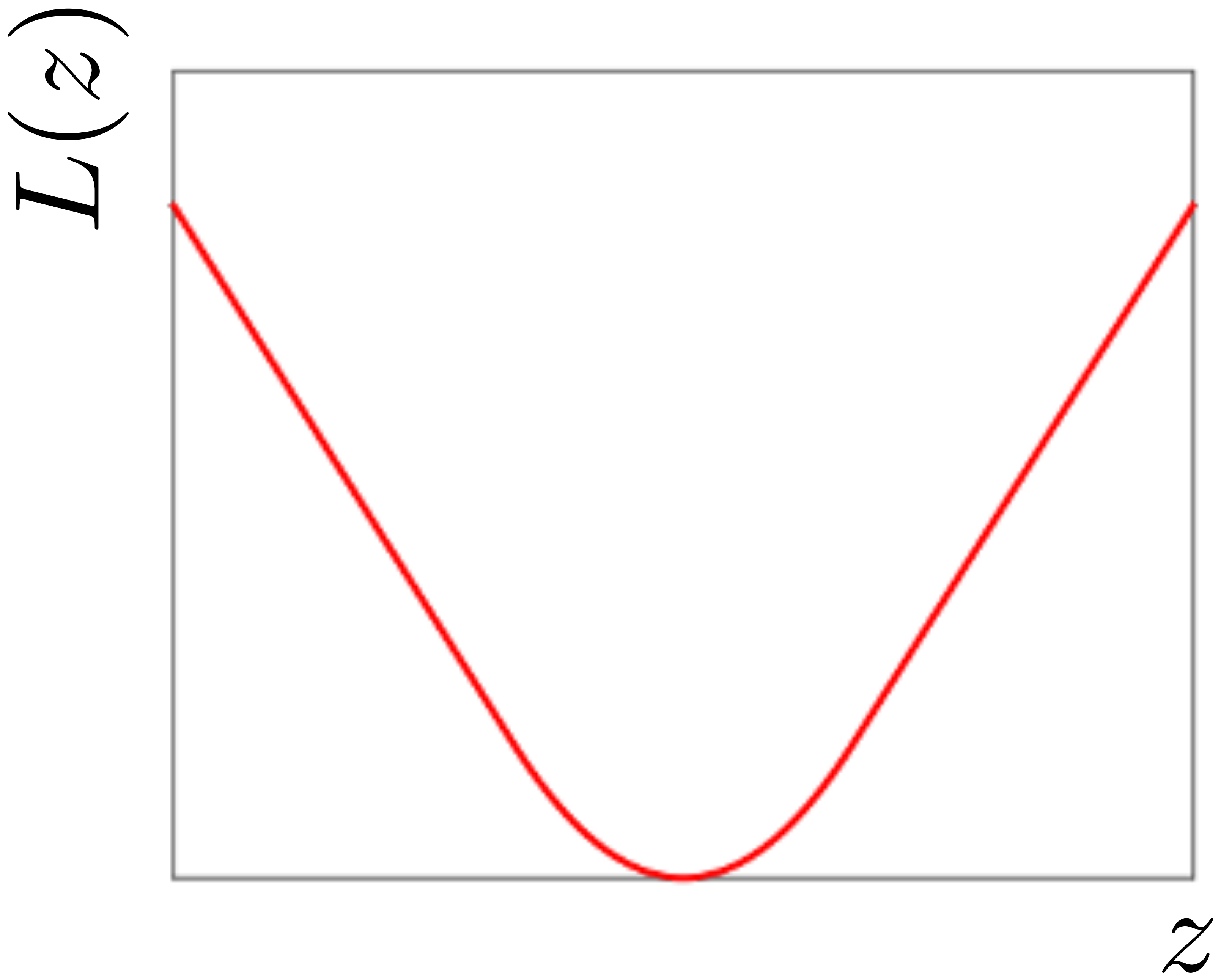
Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \dfrac{1}{N}\sum_{i=1}^{N} L(h(\widehat{x}_i) - \widehat{y}_i)$

Regression Models

Target function: $f(x) = h(x)$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \frac{1}{N}\sum_{i=1}^{N} L(h(\widehat{x}_i) - \widehat{y}_i)$

Robust Regression



Huber Loss:

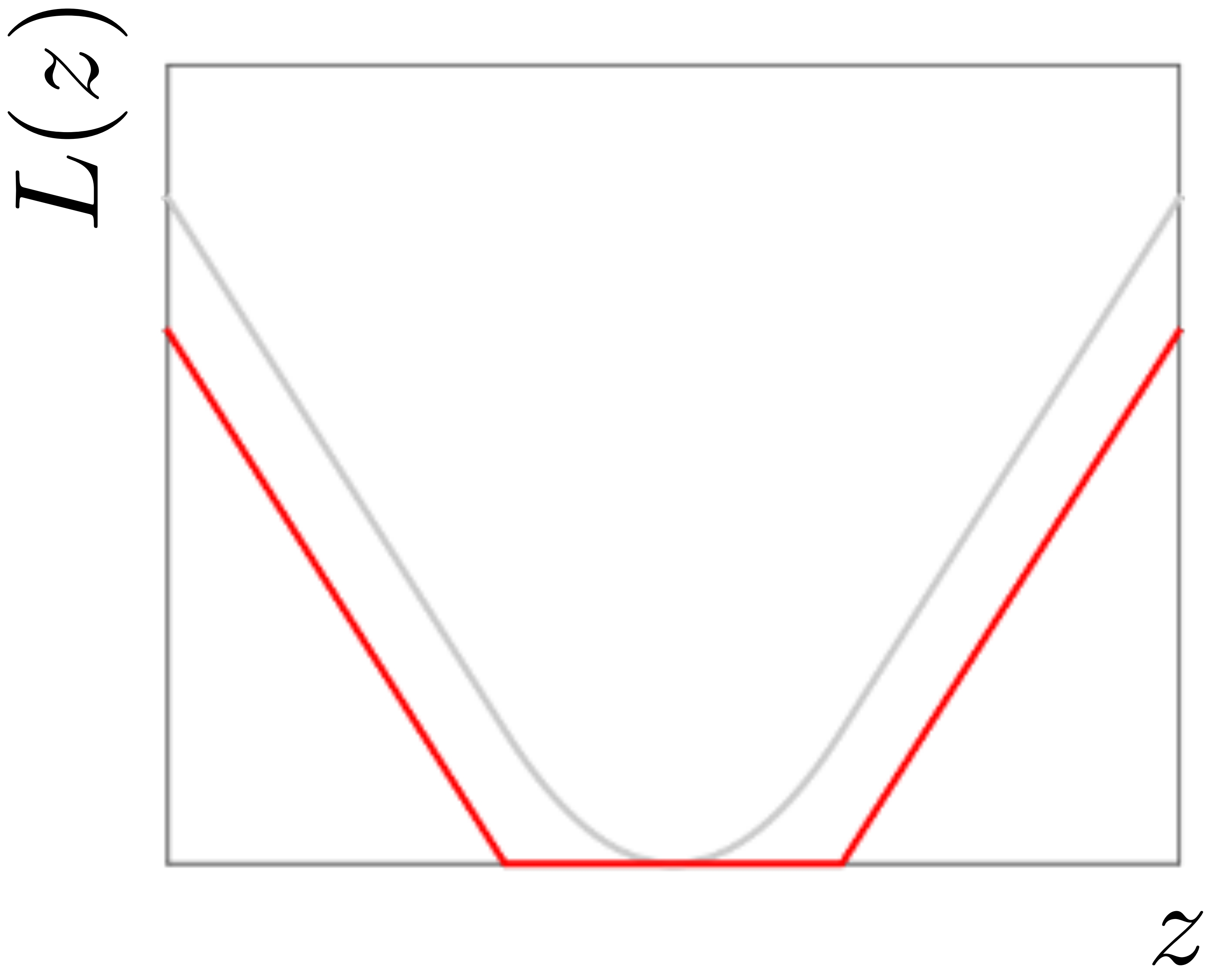
$$L(z) = \begin{cases} \frac{1}{2}z^2 & \text{if } \ |z| \leq \delta \\ \delta\left(|z| - \frac{1}{2}\delta\right) & \text{else} \end{cases}$$

Regression Models

Target function: $f(x) = h(x)$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \frac{1}{N}\sum_{i=1}^{N} L(h(\widehat{x}_i) - \widehat{y}_i)$

Support Vector Regression



ε-insensitive Loss:

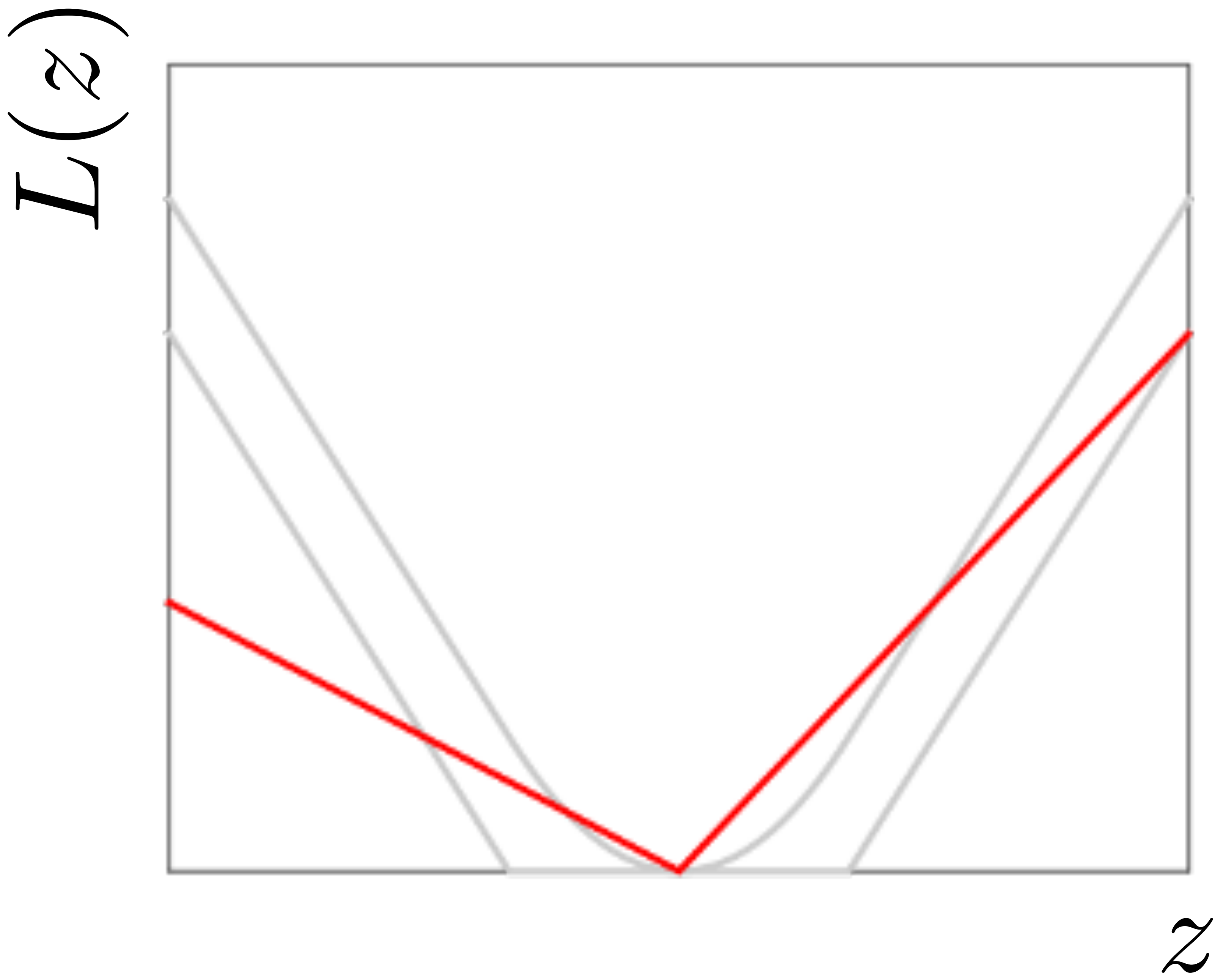
$$L(z) = \max\{0, |z| - \varepsilon\}$$

Regression Models

Target function: $f(x) = h(x)$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \frac{1}{N}\sum_{i=1}^{N} L(h(\widehat{x}_i) - \widehat{y}_i)$

Quantile Regression



Pinball Loss:

$$L(z) = \max\{-\tau z, (1-\tau)z\}$$

Classification Models

Target function: $f(x) = \mathrm{sgn}(h(x))$

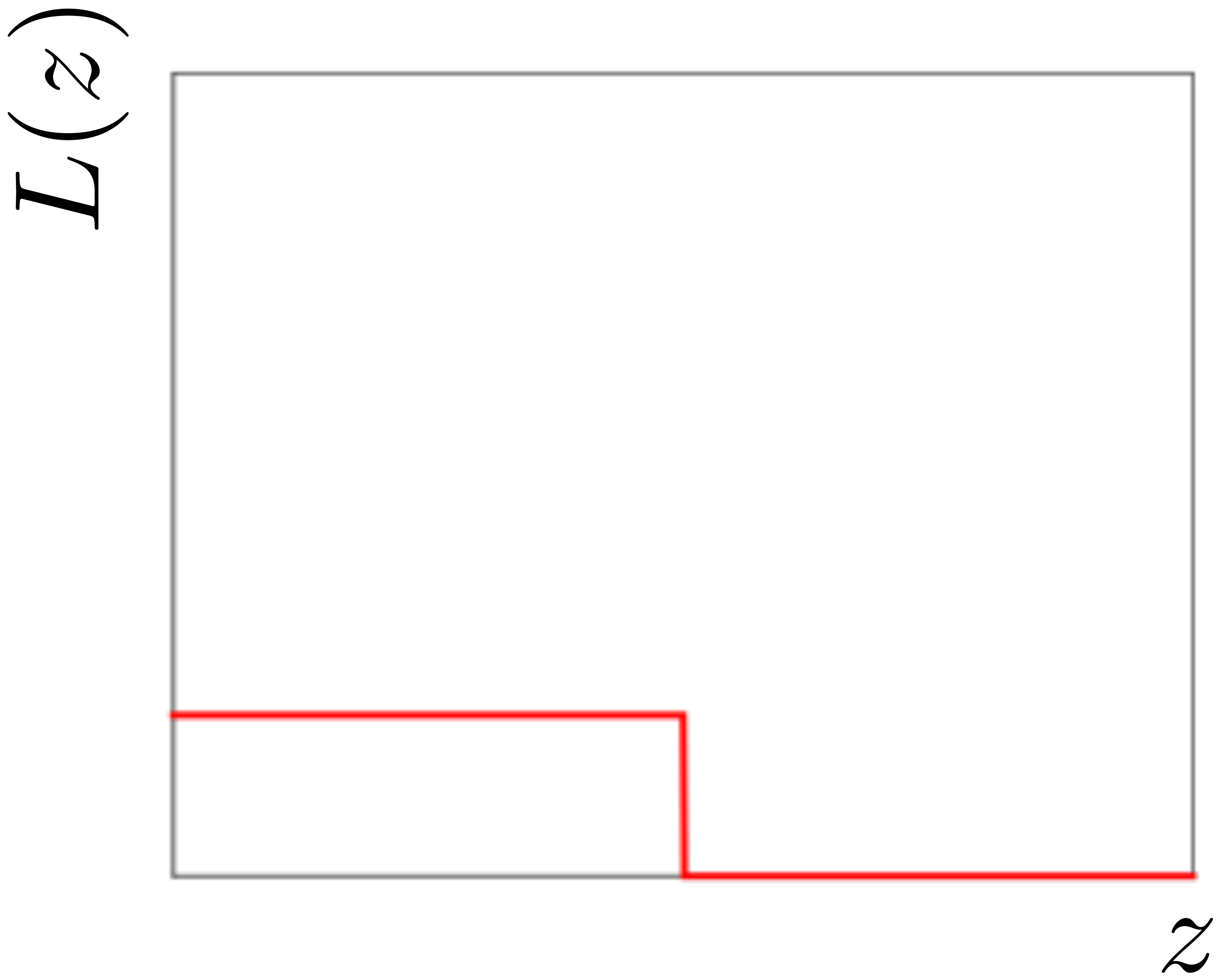
Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \dfrac{1}{N}\sum_{i=1}^{N} L(\widehat{y}_i h(\widehat{x}_i))$

Classification Models

Target function: $f(x) = \operatorname{sgn}(h(x))$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \frac{1}{N}\sum_{i=1}^{N} L(\widehat{y}_i h(\widehat{x}_i))$

Ideal Classification



0-1 Loss:

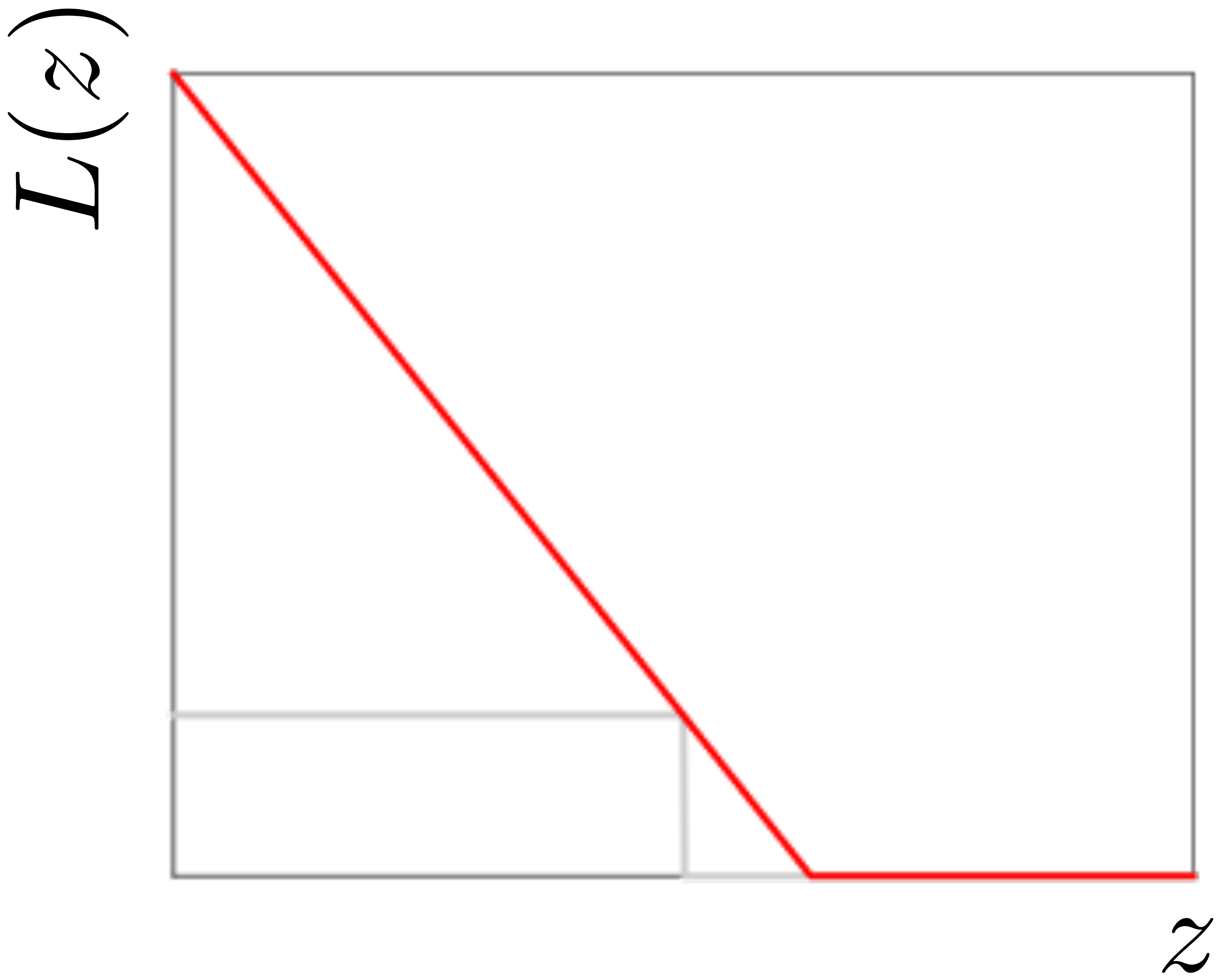
$$L(z) = \begin{cases} 1 & \text{if } z \leq 0 \\ 0 & \text{else} \end{cases}$$

Classification Models

Target function: $f(x) = \operatorname{sgn}(h(x))$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \frac{1}{N}\sum_{i=1}^{N} L(\widehat{y}_i h(\widehat{x}_i))$

Support Vector Machine



Hinge Loss:

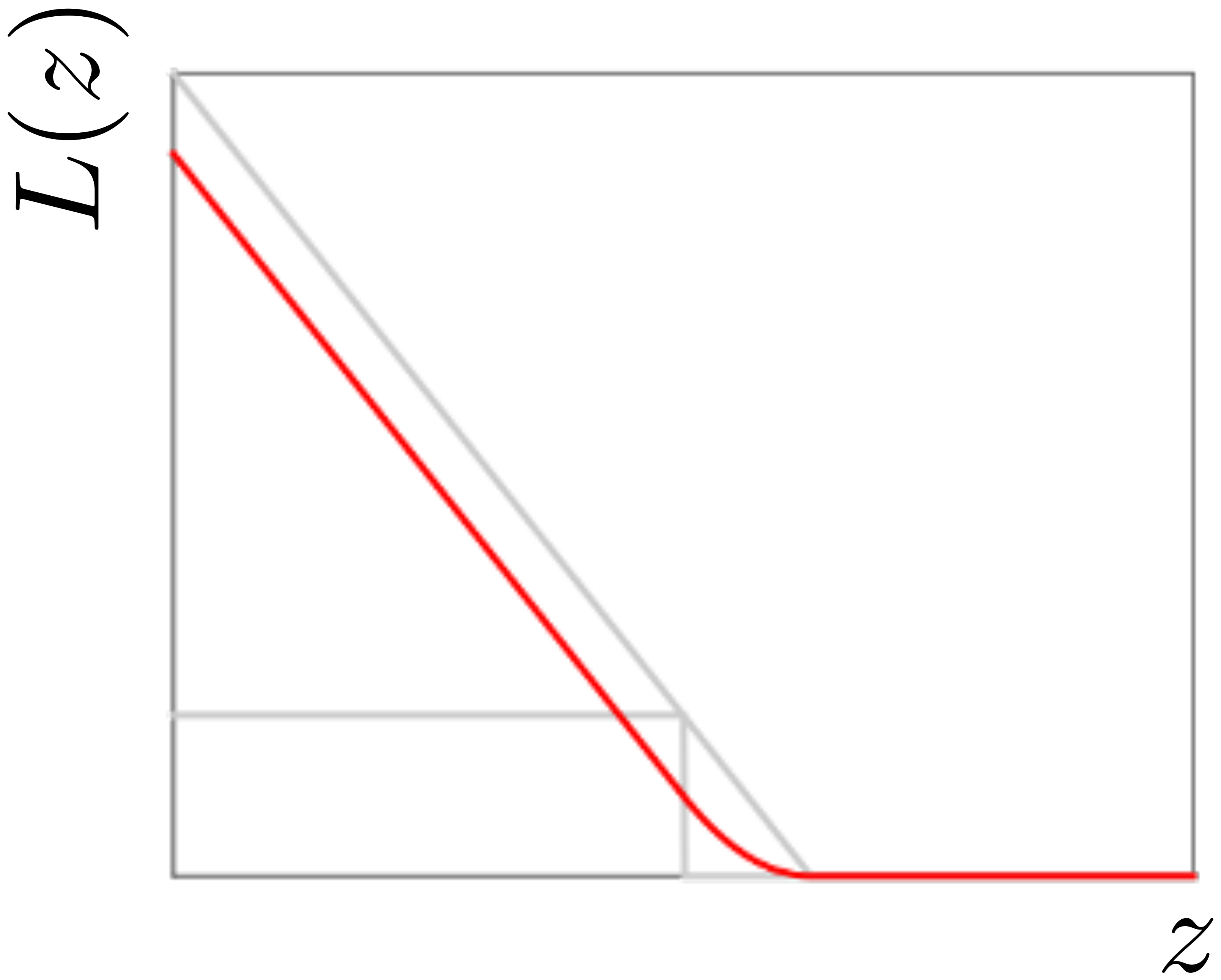
$$L(z) = \max\{0, 1 - z\}$$

Classification Models

Target function: $f(x) = \mathrm{sgn}(h(x))$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \dfrac{1}{N}\sum_{i=1}^{N} L(\widehat{y}_i h(\widehat{x}_i))$

Support Vector Machine II



Smooth Hinge Loss:

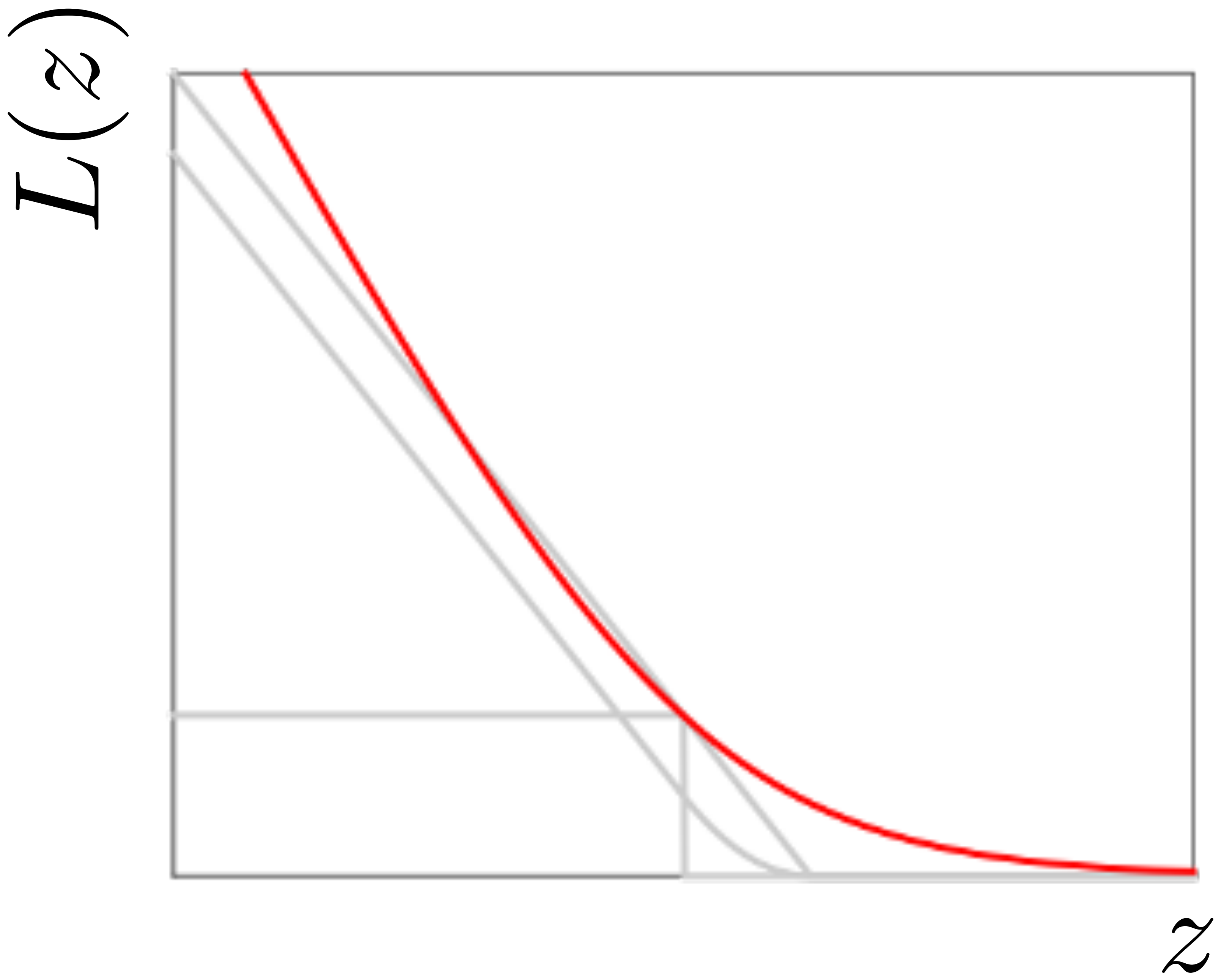
$$L(z) = \begin{cases} \frac{1}{2} - z & \text{if } z \leq 0 \\ \frac{1}{2}(1-z)^2 & \text{if } 0 < z < 1 \\ 0 & \text{else} \end{cases}$$

Classification Models

Target function: $f(x) = \mathrm{sgn}(h(x))$

Empirical risk minimization: $\ell(h, \widehat{\Xi}_N) = \frac{1}{N}\sum_{i=1}^{N} L(\widehat{y}_i h(\widehat{x}_i))$

Logistic Regression



Logloss:

$$L(z) = \log(1 + \exp(-z))$$

Performance of ERM

$$h_{\text{ERM}} = \operatorname*{argmin}_{h \in \mathbb{H}} \; \frac{1}{N} \sum_{i=1}^{N} L(h(\widehat{x}_i), \widehat{y}_i)$$

In-Sample Loss:

$$\mathbb{E}_{\widehat{\mathbb{P}}_N} \left[L(h(x), y) \right]$$

Performance of ERM

$$h_{\mathrm{ERM}} = \operatorname*{argmin}_{h \in \mathbb{H}} \ \frac{1}{N} \sum_{i=1}^{N} L(h(\widehat{x}_i), \widehat{y}_i)$$

In-Sample Loss:

$$\mathbb{E}_{\widehat{\mathbb{P}}_N} \left[L(h(x), y) \right]$$

Out-of-Sample Loss:

$$\mathbb{E}_{\mathbb{P}} \left[L(h(x), y) \right]$$

Performance of ERM

$$h_{\mathrm{ERM}} = \operatorname*{argmin}_{h \in \mathbb{H}} \; \frac{1}{N} \sum_{i=1}^{N} L(h(\widehat{x}_i), \widehat{y}_i)$$

In-Sample Loss:

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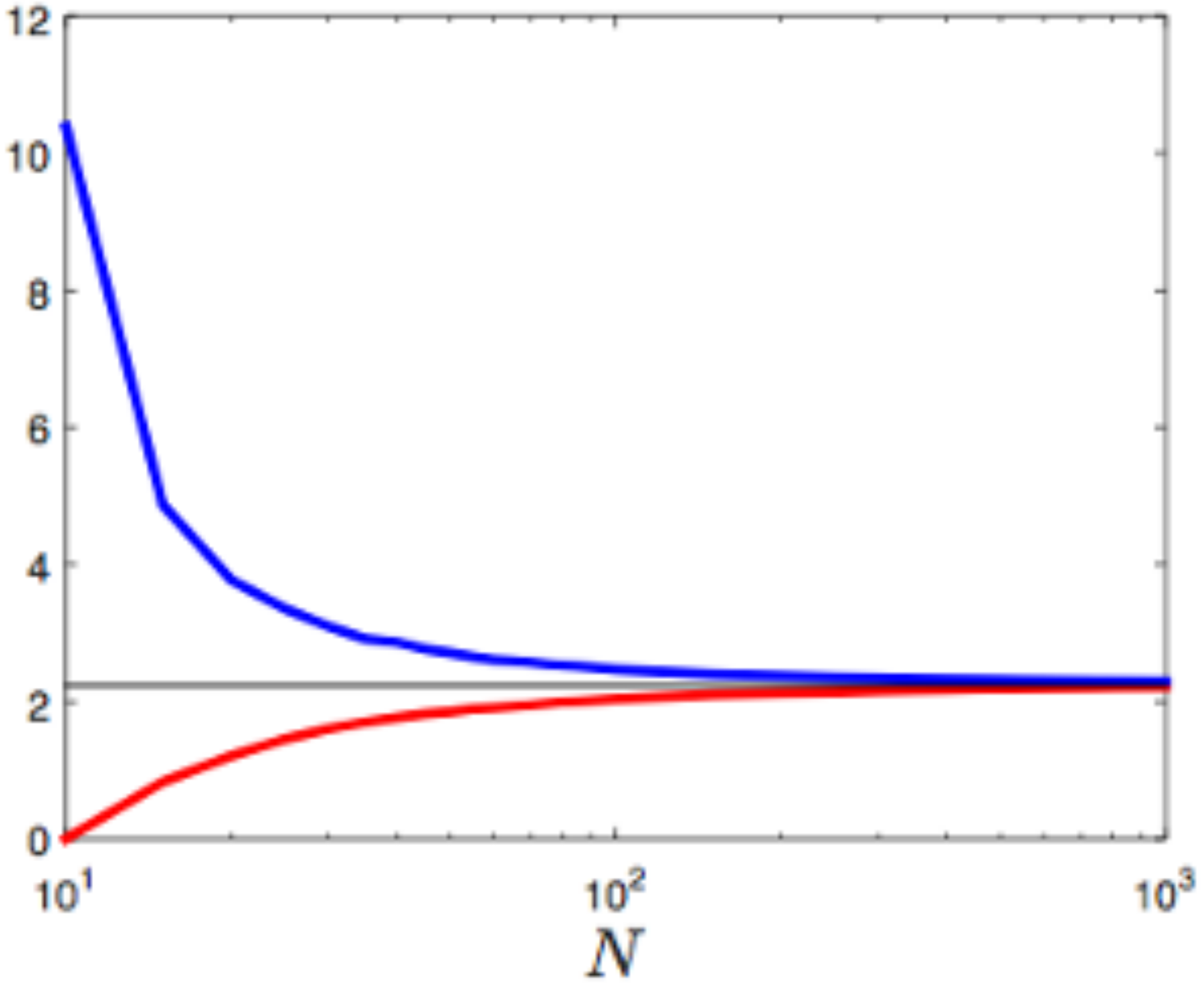
Out-of-Sample Loss:

$$\mathbb{E}_{\mathbb{P}} \left[L(h(x), y) \right]$$



Regularized ERM

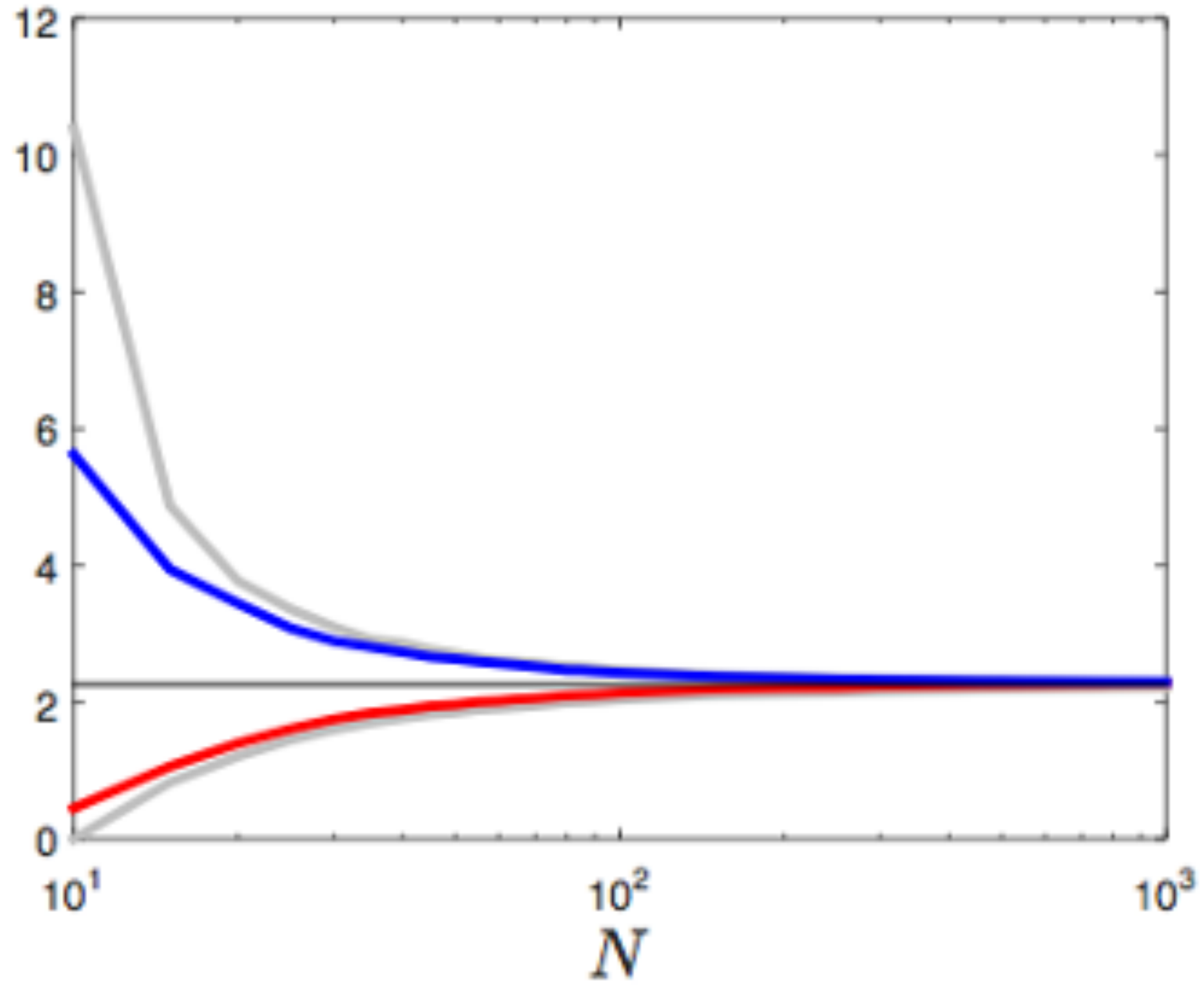
$$h_{\text{REG}} = \operatorname*{argmin}_{h \in \mathbb{H}} \frac{1}{N} \sum_{i=1}^{N} L(h(\widehat{x}_i), \widehat{y}_i) + \underbrace{\varepsilon}_{\text{Regularization coefficient}} \underbrace{\Omega(h)}_{\text{Regularization function}}$$

Regularized ERM

$$h_{\text{REG}} = \operatorname*{argmin}_{h \in \mathbb{H}} \frac{1}{N} \sum_{i=1}^{N} L(h(\widehat{x}_i), \widehat{y}_i) + \varepsilon \, \Omega(h)$$

Regularization coefficient

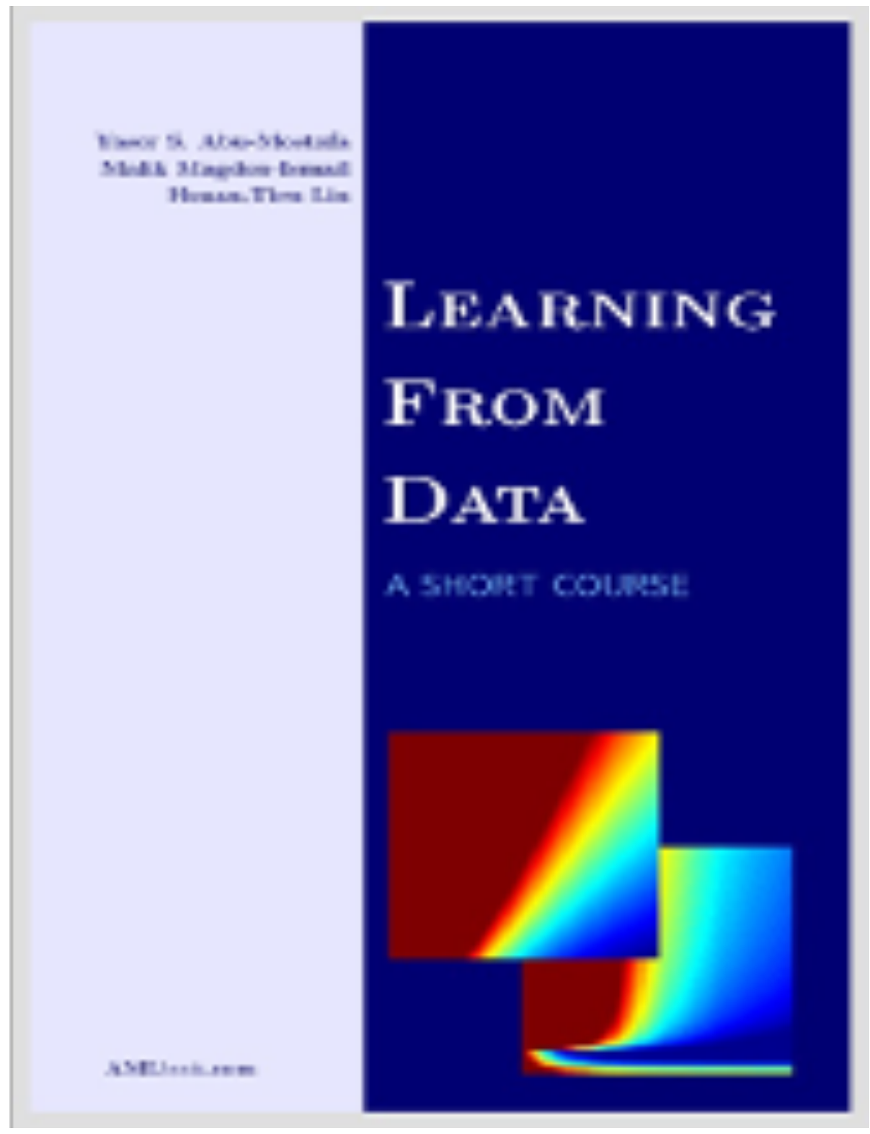
Regularization function



Regularized ERM

> “Most of the **regularization methods** used successfully in practice **are heuristic methods**.”

Abu-Mostafa *et al.*, 2012.



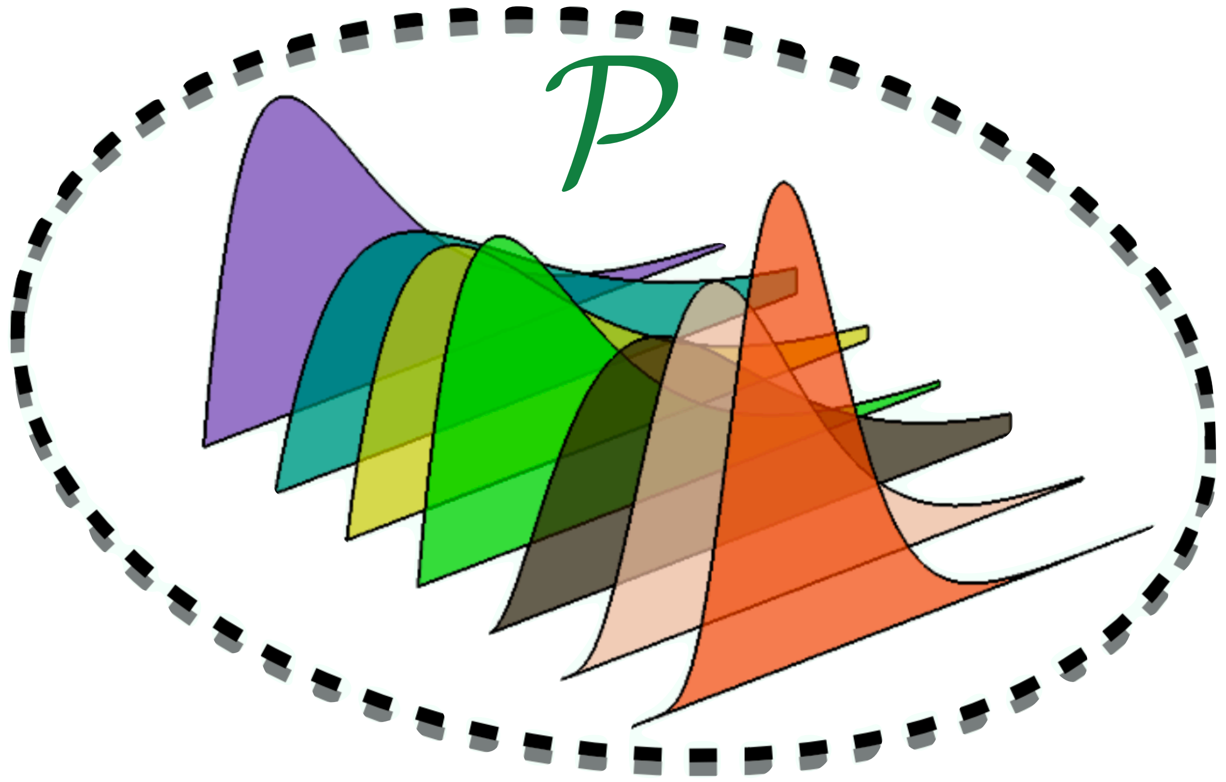
LEARNING FROM DATA

A SHORT COURSE

Regularization via Optimal Transport

$$\inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(h(x), y) \right]$$

$$\mathbb{H} = \left\{ h \in \mathbb{R}^{\mathbb{X}} : \exists \theta \in \boldsymbol{\Theta} \text{ s.t. } h(x) = \theta^\top x \right\}$$



Regularization via Optimal Transport

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x, y) \right]$$

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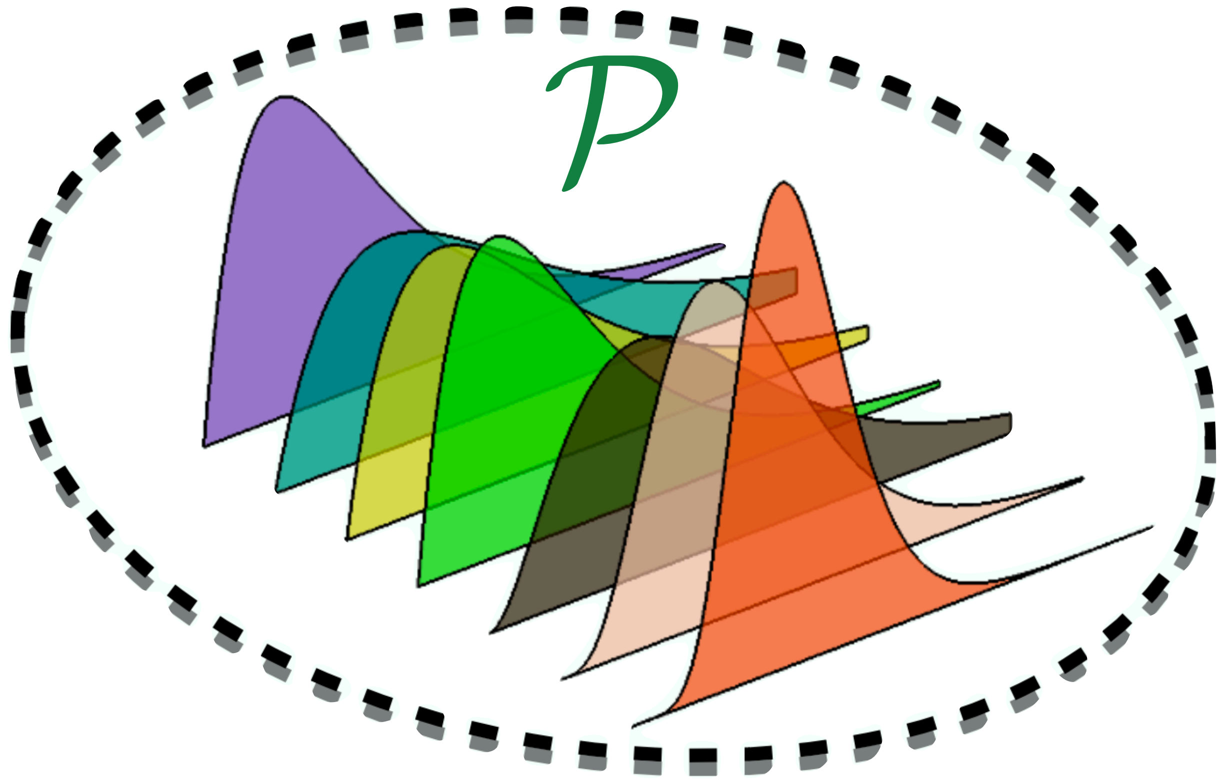


The Real Story Behind the Success

Regularization

[SMK15, GCK17, CP18, BMZ18, BKM19, SKM19]

Statistical Guarantees

[SMK15, MK18, BKM19, SKM19, G20, BMN21]

Optimal Transport: Old and New

Monge **Hitchcock** **Kantorovich-Koopmans** **Vaserstein** **Brenier** **Villani** **Figalli**

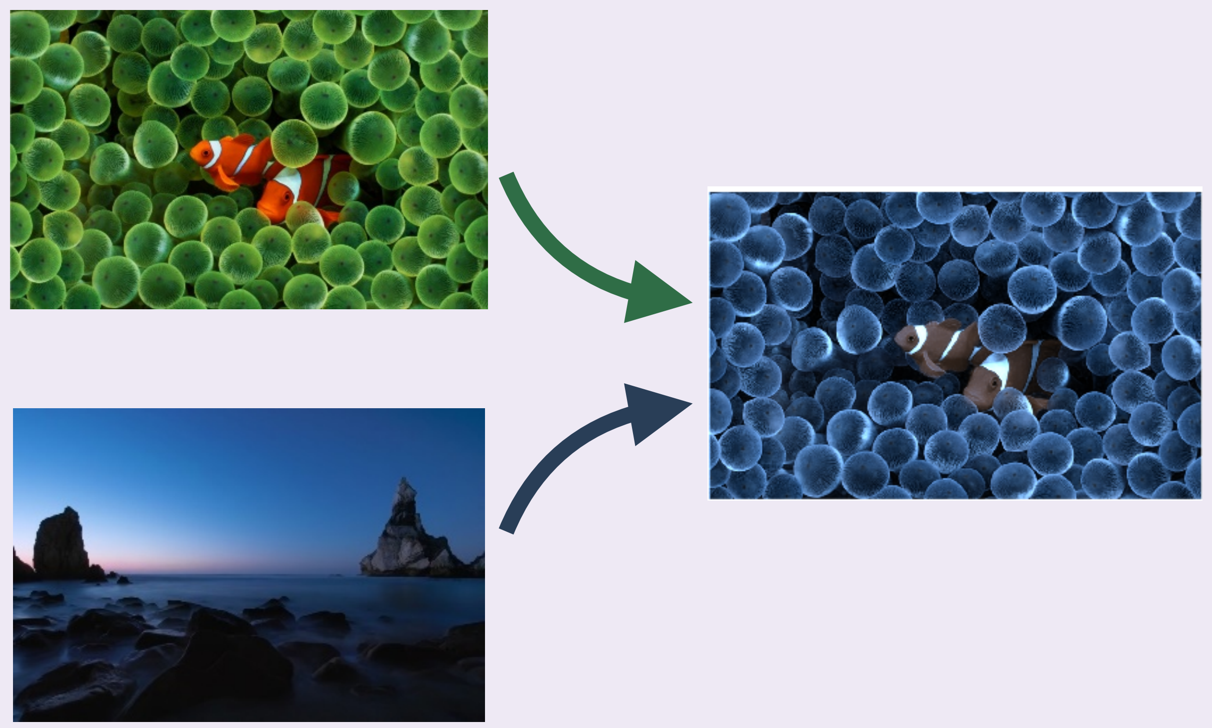
Nobel ‘75

Fields ‘10

Fields ‘18

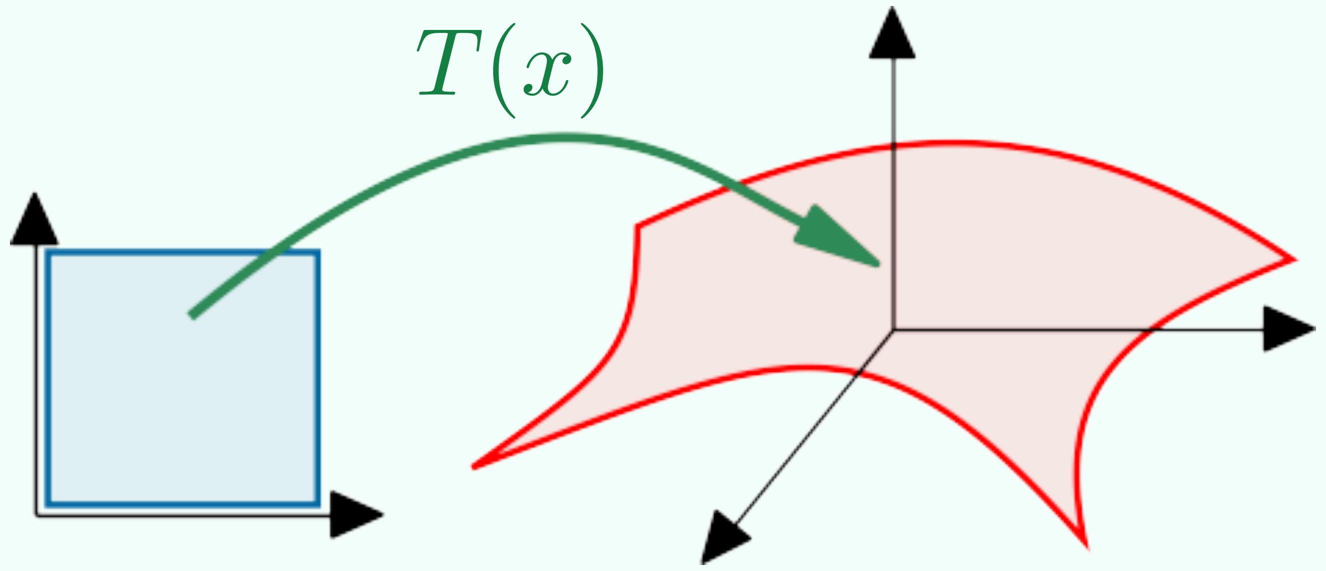
Applications

Color Histogram [PPC10]



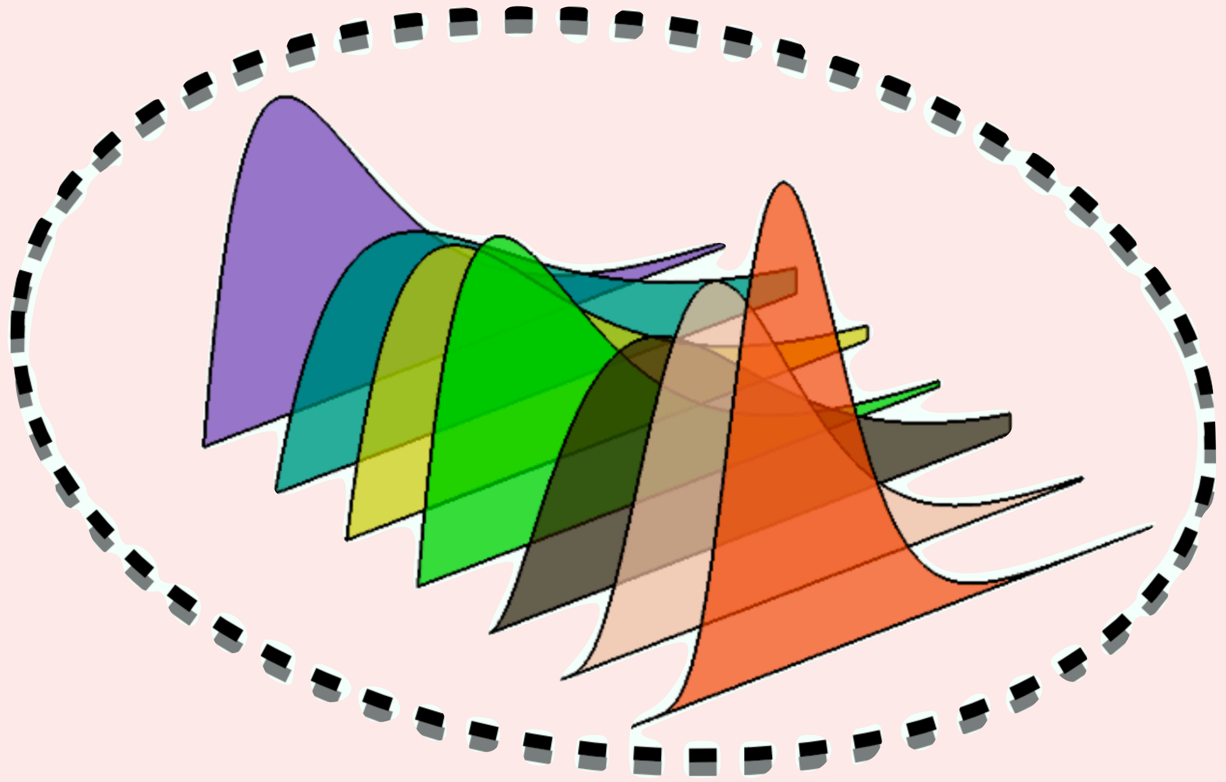
Computer Graphics [LS18]

Generative Models [ACB17]



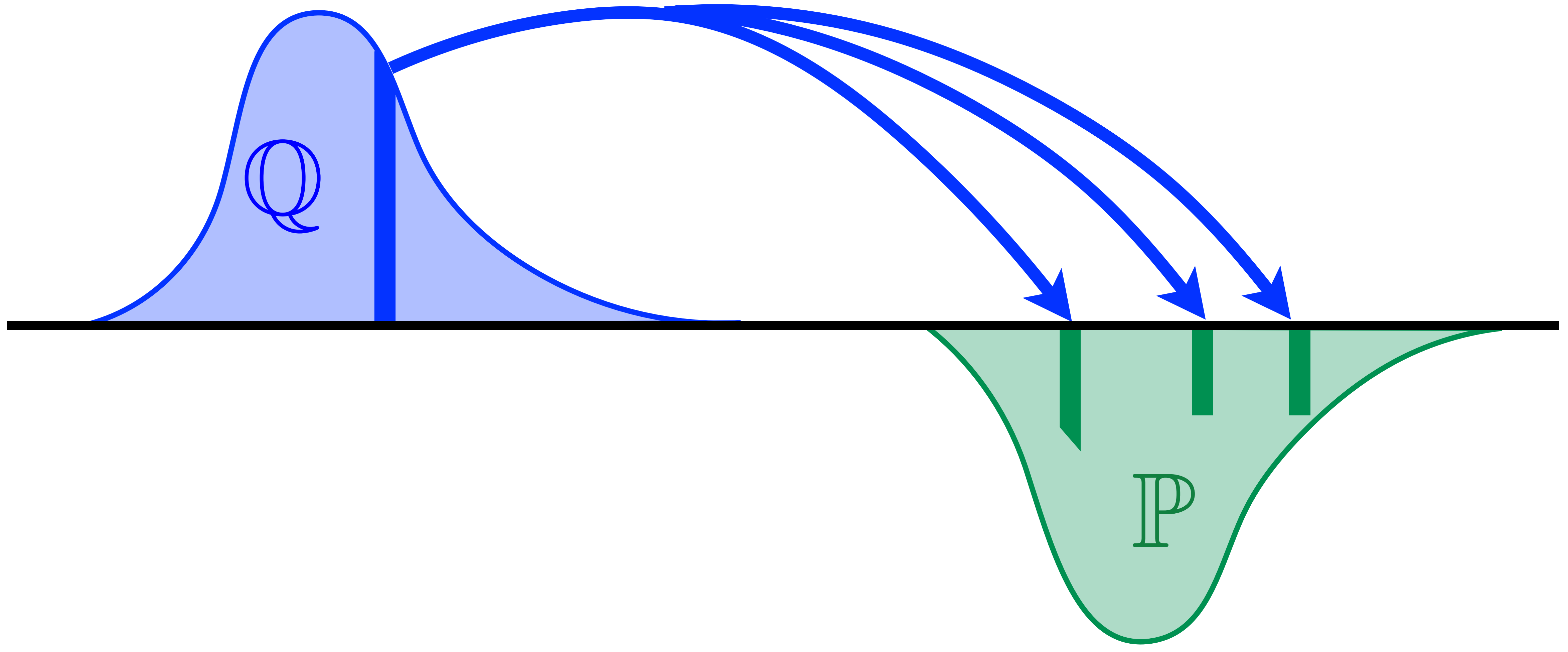
Finance and Economics [Gal16]

Statistical Inference



Text Classification [HGKSSW16]

What is Optimal Transport?

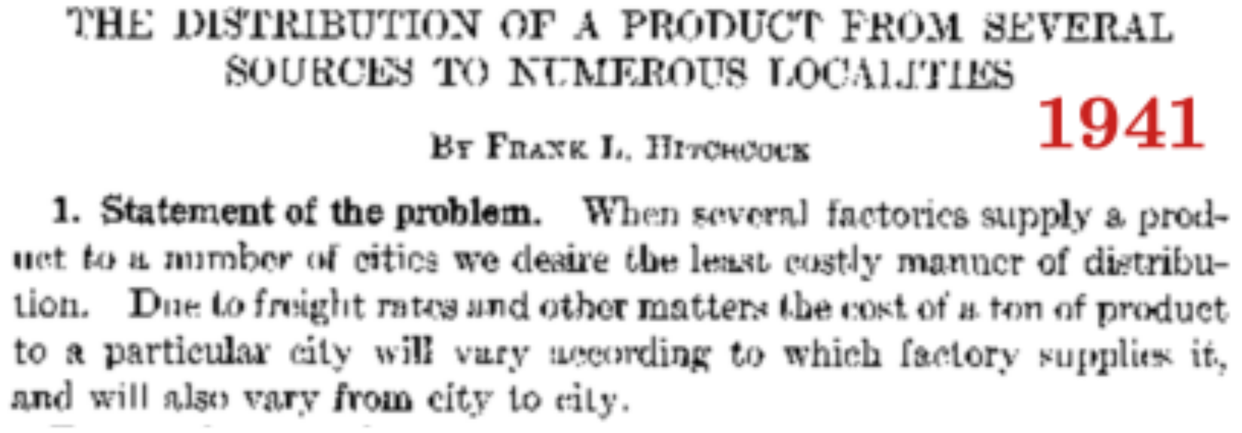


$$W_c(\mathbb{Q},\mathbb{P}) = \begin{cases} \inf\limits_{\pi\in\mathcal{M}(\Xi,\Xi)} & \mathbb{E}_\pi\left[c(\xi,\xi')\right] \\ \text{s.t.} & \pi\in\Pi(\mathbb{Q},\mathbb{P}) \end{cases}$$

проф. Л. В. КАНТОРОВИЧ

1939

МАТЕМАТИЧЕСКИЕ
МЕТОДЫ
ОРГАНИЗАЦИИ
И ПЛАНИРОВАНИЯ
ПРОИЗВОДСТВА

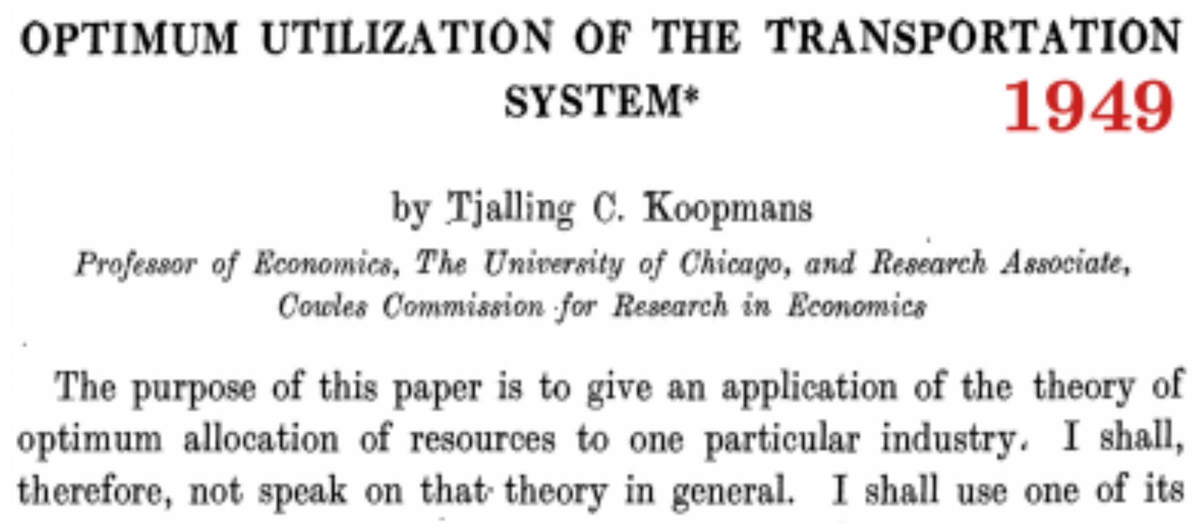


THE DISTRIBUTION OF A PRODUCT FROM SEVERAL SOURCES TO NUMEROUS LOCALITIES

1941

By Frank L. Hitchcock

1. Statement of the problem. When several factories supply a product to a number of cities we desire the least costly manner of distribution. Due to freight rates and other matters the cost of a ton of product to a particular city will vary according to which factory supplies it, and will also vary from city to city.



OPTIMUM UTILIZATION OF THE TRANSPORTATION SYSTEM*

1949

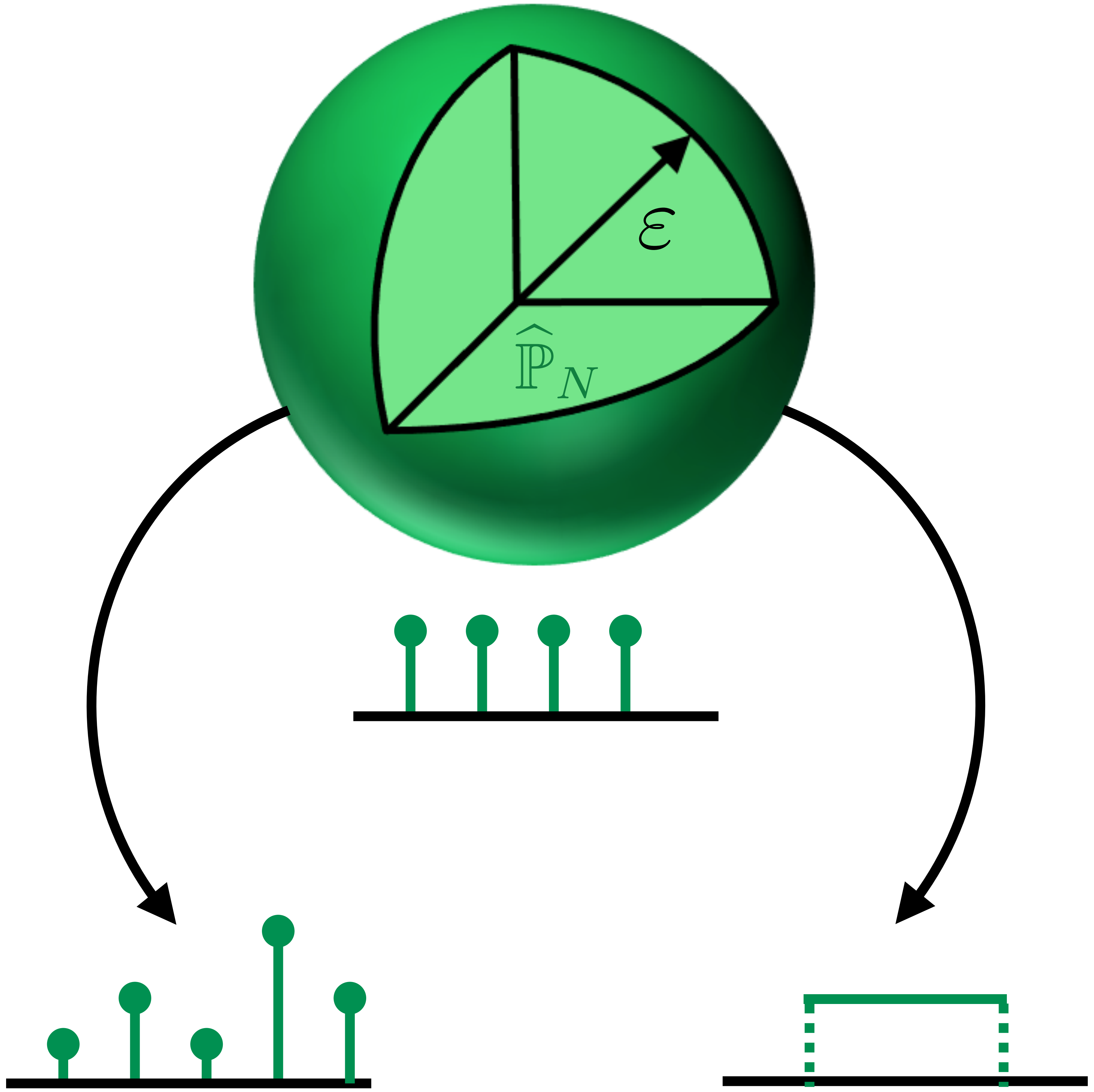
by Tjalling C. Koopmans

Professor of Economics, The University of Chicago, and Research Associate, Cowles Commission for Research in Economics

The purpose of this paper is to give an application of the theory of optimum allocation of resources to one particular industry. I shall, therefore, not speak on that theory in general. I shall use one of its

Optimal Transport Ambiguity Set

$$\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\mathbb{R}^n \times \mathbb{Y}) : W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N) \leq \varepsilon\}$$



Optimal Transport Ambiguity Set

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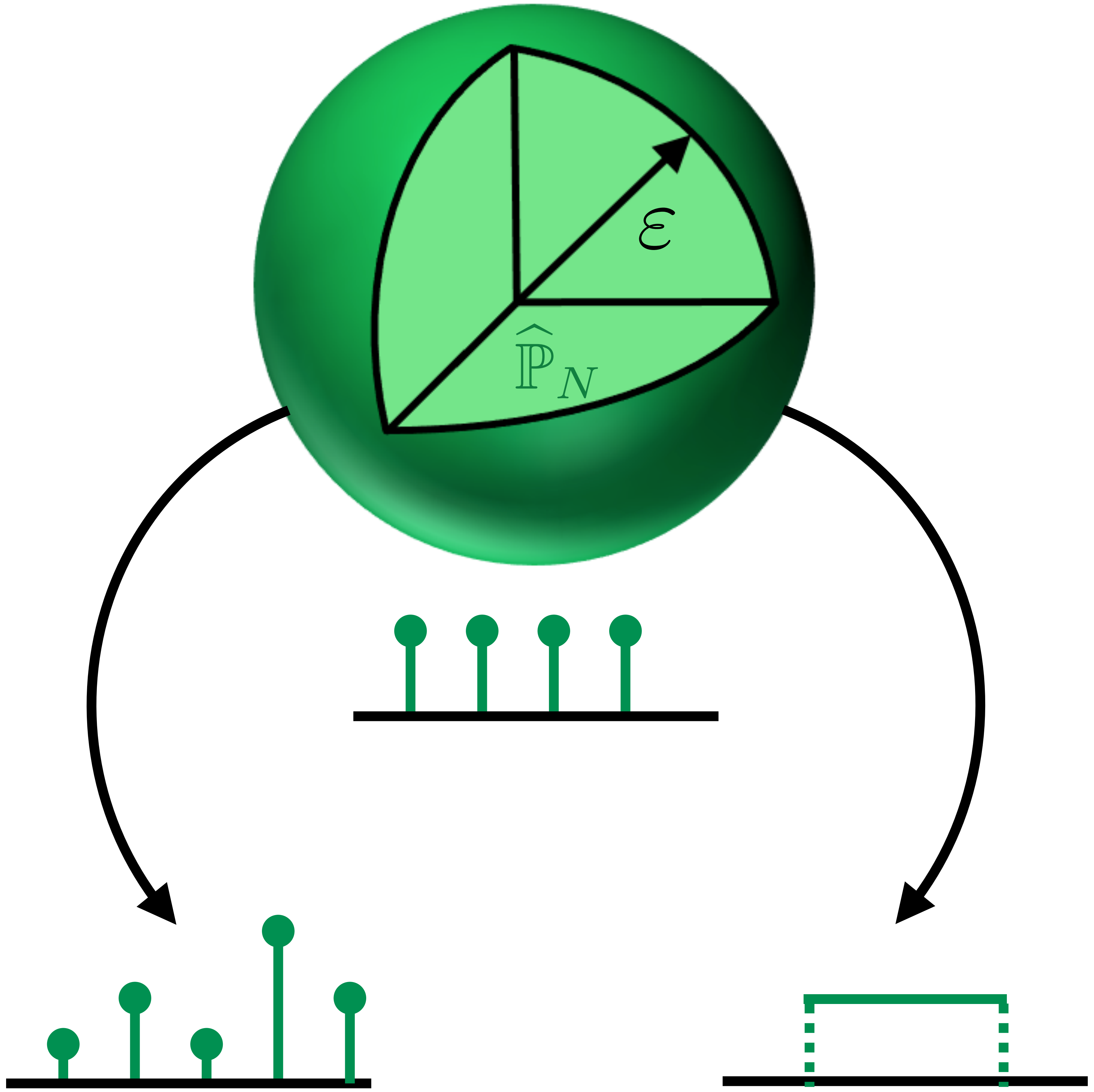
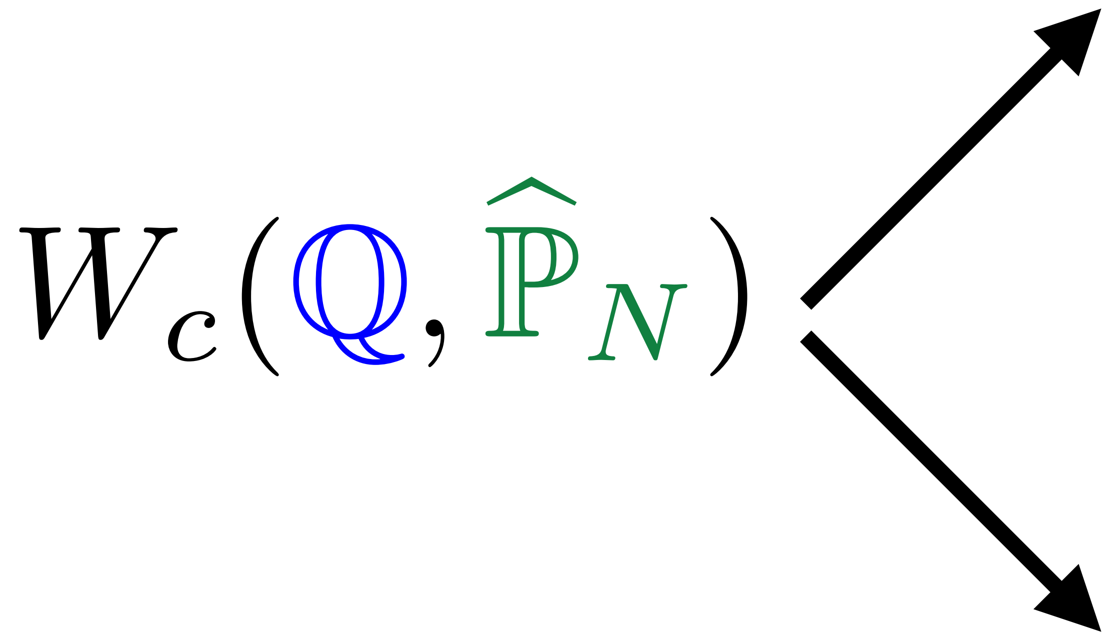




$W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N)$

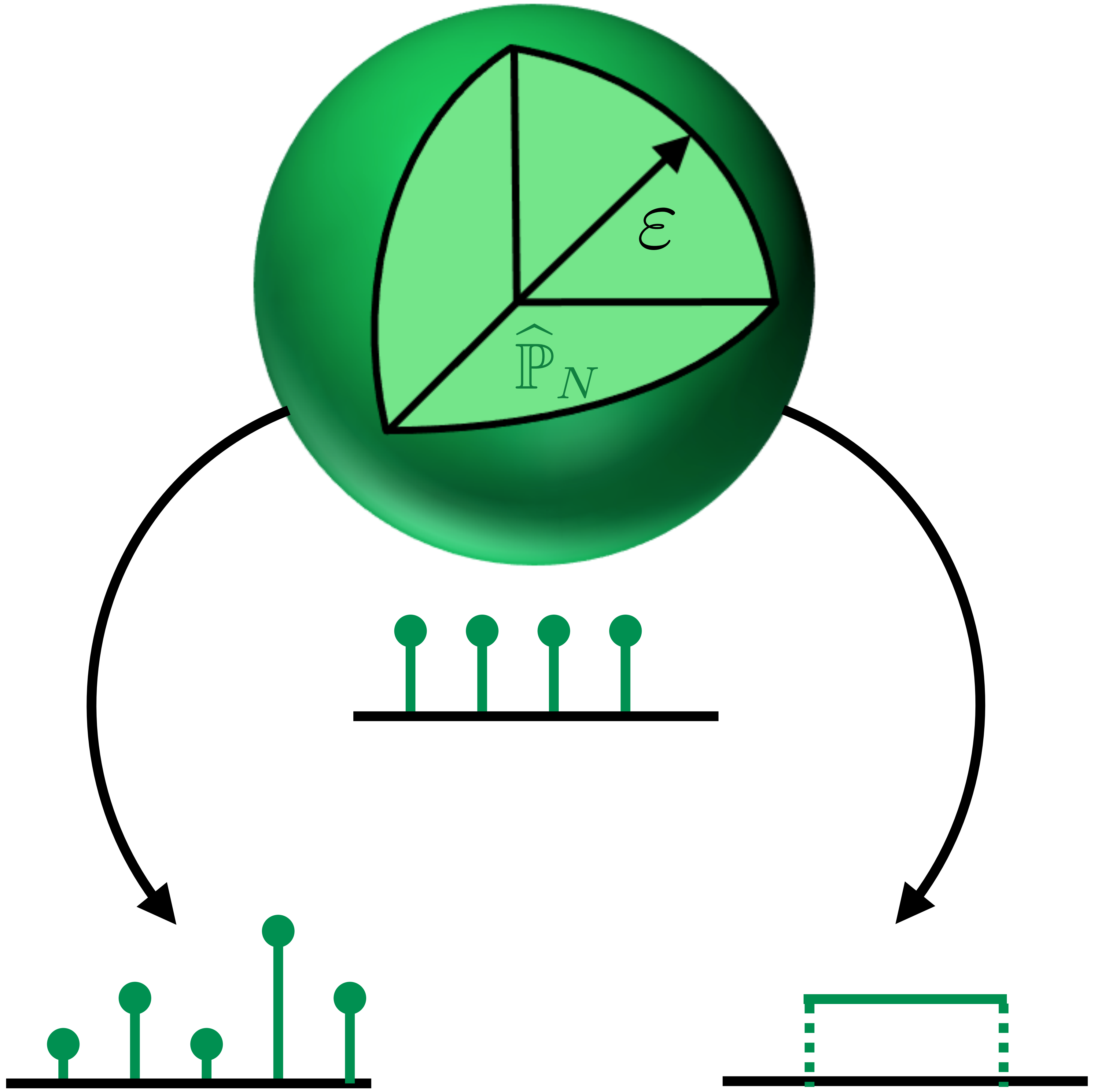
discrete OT is easy!

semi-discrete OT is hard!

[TSK2022]

Optimal Transport Ambiguity Set

$$\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\mathbb{R}^n \times \mathbb{Y}) : W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N) \leq \varepsilon\}$$



$$\begin{aligned} \sup_{\mathbb{Q} \in \mathcal{M}(\Xi)} \quad & \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x, y)\right] \\ \text{s.t.} \quad & W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N) \leq \varepsilon \end{aligned}$$

Tractability for Linear Regression

Theorem 1. Suppose that $c\big((x, y), (x', y')\big) = \|x - x'\| + \delta_{y=y'}$.

If L is convex and Lipschitz, then

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right] = \inf_{\theta \in \Theta} \frac{1}{N} \sum_{i=1}^{N} L(\theta^\top \widehat{x}_i - \widehat{y}_i) + \varepsilon \mathrm{lip}(L) \|\theta\|_*$$

[SMK15, GCK17, SKM19, BKM19]

Tractability for Linear Regression

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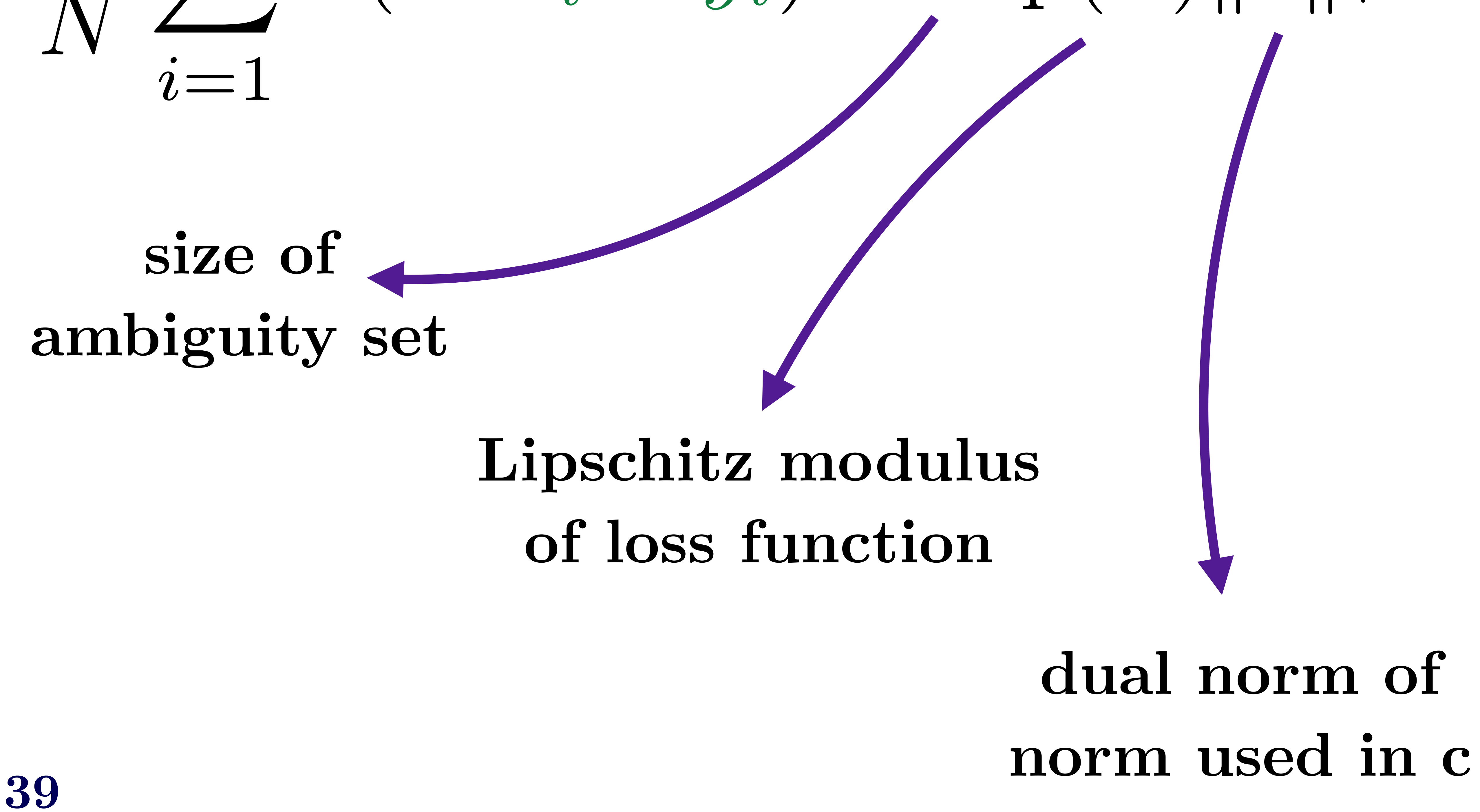


size of ambiguity set

Lipschitz modulus of loss function

dual norm of norm used in c

[SMK15, GCK17, SKM19, BKM19]

Semi-infinite Duality

Lemma 1. Let $\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\Xi) : W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N) \leq \varepsilon\}$. If $c(\xi, \xi) = 0$ for all $\xi \in \Xi$ and $\varepsilon > 0$, then

$$\sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}}[I(\xi)] = \inf_{\lambda \geq 0} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{\zeta \in \Xi} I(\zeta) - \lambda c(\zeta, \xi)\right]$$

[MK18, ZG18, BM19, GK16, ZYG22]

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] = \left\{ \begin{array}{cl} \sup\limits_{\mathbb{Q}\in\mathcal{M}(\Xi)} & \displaystyle\int_{\xi\in\Xi} I(\xi)\mathbb{Q}(\mathrm{d}\xi) \\ \text{s.t.} & W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N) \leq \varepsilon \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] = \left\{ \begin{array}{cl} \sup\limits_{\mathbb{Q}\in\mathcal{M}(\Xi)} & \displaystyle\int_{\xi\in\Xi} I(\xi)\mathbb{Q}(\mathrm{d}\xi) \\[2em] \text{s.t.} & W_c(\mathbb{Q},\widehat{\mathbb{P}}_N) \leq \varepsilon \end{array} \right.$$

$$= \left\{ \begin{array}{cl} \sup\limits_{\substack{\mathbb{Q}\in\mathcal{M}(\Xi)\\ \pi\in\mathcal{M}(\Xi\times\Xi)}} & \displaystyle\int_{\xi\in\Xi} I(\xi)\mathbb{Q}(\mathrm{d}\xi) \\[2em] \text{s.t.} & \pi \in \Pi(\mathbb{Q},\widehat{\mathbb{P}}_N) \\[2em] & \displaystyle\int_{\xi\in\Xi}\int_{\xi'\in\Xi} c(\xi,\xi')\pi(\mathrm{d}\xi,\mathrm{d}\xi') \leq \varepsilon \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] = \left\{ \begin{array}{cl} \sup\limits_{\mathbb{Q}\in\mathcal{M}(\Xi)} & \displaystyle\int_{\xi\in\Xi} I(\xi)\mathbb{Q}(\mathrm{d}\xi) \\ \text{s.t.} & W_c(\mathbb{Q},\widehat{\mathbb{P}}_N) \leq \varepsilon \end{array} \right.$$

$$W_c(\mathbb{Q},\widehat{\mathbb{P}}_N) = \left\{ \begin{array}{cl} \inf\limits_{\pi\in\mathcal{M}(\Xi,\Xi)} & \mathbb{E}_\pi\left[c(\xi,\xi')\right] \\ \text{s.t.} & \pi\in\Pi(\mathbb{Q},\widehat{\mathbb{P}}_N) \end{array} \right.$$

$$= \left\{ \begin{array}{cl} \sup\limits_{\substack{\mathbb{Q}\in\mathcal{M}(\Xi)\\ \pi\in\mathcal{M}(\Xi\times\Xi)}} & \displaystyle\int_{\xi\in\Xi} I(\xi)\mathbb{Q}(\mathrm{d}\xi) \\ \text{s.t.} & \pi\in\Pi(\mathbb{Q},\widehat{\mathbb{P}}_N) \\ & \displaystyle\int_{\xi\in\Xi}\int_{\xi'\in\Xi} c(\xi,\xi')\pi(\mathrm{d}\xi,\mathrm{d}\xi') \leq \varepsilon \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] = \begin{cases} \sup\limits_{\mathbb{Q}_i\in\mathcal{M}(\Xi)} & \dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\int_{\xi\in\Xi} I(\xi)\mathbb{Q}_i(\mathrm{d}\xi) \\ & \dfrac{1}{N}\displaystyle\int_{\xi\in\Xi} c(\xi,\widehat{\xi}_i)\mathbb{Q}_i(\mathrm{d}\xi) \leq \varepsilon \end{cases}$$

$$\boxed{\begin{cases} \pi \in \Pi(\mathbb{Q},\widehat{\mathbb{P}}_N) \\ \widehat{\mathbb{P}}_N = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\delta_{\widehat{\xi}_i} \end{cases} \Longrightarrow \begin{cases} \pi = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\mathbb{Q}_i \times \delta_{\widehat{\xi}_i} \\ \mathbb{Q} = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\mathbb{Q}_i \end{cases}}$$

Proof of Lemma 1

$$\sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} [I(\xi)] = \left\{ \begin{array}{ll} \sup\limits_{\mathbb{Q}_i \in \mathcal{M}(\Xi)} & \dfrac{1}{N} \sum\limits_{i=1}^{N} \int_{\xi \in \Xi} I(\xi) \mathbb{Q}_i(\mathrm{d}\xi) \\ & \dfrac{1}{N} \int_{\xi \in \Xi} c(\xi, \widehat{\xi}_i) \mathbb{Q}_i(\mathrm{d}\xi) \le \varepsilon \end{array} \right.$$

$$\boxed{\begin{cases} \pi \in \Pi(\mathbb{Q}, \widehat{\mathbb{P}}_N) \\ \widehat{\mathbb{P}}_N = \dfrac{1}{N} \sum\limits_{i=1}^{N} \delta_{\widehat{\xi}_i} \end{cases} \Longrightarrow \begin{cases} \pi = \dfrac{1}{N} \sum\limits_{i=1}^{N} \mathbb{Q}_i \times \delta_{\widehat{\xi}_i} \\ \mathbb{Q} = \dfrac{1}{N} \sum\limits_{i=1}^{N} \mathbb{Q}_i \end{cases}}$$

$$= \left\{ \begin{array}{ll} \sup\limits_{\mathbb{Q}_i \ge 0} & \dfrac{1}{N} \sum\limits_{i=1}^{N} \int_{\xi \in \Xi} I(\xi) \mathbb{Q}_i(\mathrm{d}\xi) \\ & \dfrac{1}{N} \int_{\xi \in \Xi} c(\xi, \widehat{\xi}_i) \mathbb{Q}_i(\mathrm{d}\xi) \le \varepsilon \\ & \int_{\xi \in \Xi} \mathbb{Q}_i(\mathrm{d}\xi) = 1 \qquad \forall i \in [N] \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] = \left\{ \begin{array}{ll} \sup\limits_{\mathbb{Q}_i \in \mathcal{M}(\Xi)} & \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} \int_{\xi\in\Xi} I(\xi)\mathbb{Q}_i(\mathrm{d}\xi) \\ & \dfrac{1}{N}\displaystyle\int_{\xi\in\Xi} c(\xi,\widehat{\xi}_i)\mathbb{Q}_i(\mathrm{d}\xi) \leq \varepsilon \end{array} \right.$$

$$\boxed{\begin{cases} \pi \in \Pi(\mathbb{Q}, \widehat{\mathbb{P}}_N) \\ \widehat{\mathbb{P}}_N = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} \delta_{\widehat{\xi}_i} \end{cases} \Longrightarrow \begin{cases} \pi = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} \mathbb{Q}_i \times \delta_{\widehat{\xi}_i} \\ \mathbb{Q} = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} \mathbb{Q}_i \end{cases}}$$

$$= \left\{ \begin{array}{ll} \sup\limits_{\mathbb{Q}_i \geq 0} & \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} \int_{\xi\in\Xi} I(\xi)\mathbb{Q}_i(\mathrm{d}\xi) \\ & \dfrac{1}{N}\displaystyle\int_{\xi\in\Xi} c(\xi,\widehat{\xi}_i)\mathbb{Q}_i(\mathrm{d}\xi) \leq \varepsilon \qquad (\lambda) \\ & \displaystyle\int_{\xi\in\Xi} \mathbb{Q}_i(\mathrm{d}\xi) = 1 \qquad (s_i) \qquad \forall i \in [N] \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \ \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] \leq \left\{ \begin{array}{ll} \displaystyle\inf_{\substack{\lambda\geq 0 \\ s\in\mathbb{R}^N}} & \displaystyle\lambda\varepsilon + \sum_{i=1}^{N} s_i \\[2em] \text{s.t.} & \displaystyle\frac{\lambda}{N} c(\xi, \widehat{\xi}_i) + s_i \geq \frac{1}{N} I(\xi) \quad \forall \xi \in \Xi \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}[I(\xi)] \leq \left\{ \begin{array}{ll} \inf\limits_{\substack{\lambda\geq 0\\ s\in\mathbb{R}^N}} & \lambda\varepsilon + \sum\limits_{i=1}^{N} s_i \\ \text{s.t.} & \dfrac{\lambda}{N} c(\xi, \widehat{\xi}_i) + s_i \geq \dfrac{1}{N} I(\xi) \quad \forall \xi \in \Xi \end{array} \right.$$

$$= \left\{ \begin{array}{ll} \inf\limits_{\substack{\lambda\geq 0\\ s\in\mathbb{R}^N}} & \lambda\varepsilon + \sum\limits_{i=1}^{N} s_i \\ \text{s.t.} & s_i \geq \sup\limits_{\xi\in\Xi} \dfrac{1}{N} I(\xi) - \dfrac{\lambda}{N} c(\xi, \widehat{\xi}_i) \end{array} \right.$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \; \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] \leq \left\{ \begin{array}{ll} \inf\limits_{\substack{\lambda\geq 0\\ s\in\mathbb{R}^N}} & \lambda\varepsilon + \sum\limits_{i=1}^{N} s_i \\ \\ \text{s.t.} & \dfrac{\lambda}{N} c(\xi,\widehat{\xi}_i) + s_i \geq \dfrac{1}{N} I(\xi) \quad \forall \xi \in \Xi \end{array} \right.$$

$$= \inf_{\lambda\geq 0} \; \lambda\varepsilon + \frac{1}{N}\sum_{i=1}^{N} \sup_{\xi\in\Xi} \; I(\xi) - \lambda c(\xi,\widehat{\xi}_i)$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] \leq \left\{ \begin{array}{ll} \inf\limits_{\substack{\lambda\geq 0 \\ s\in\mathbb{R}^N}} & \lambda\varepsilon + \sum\limits_{i=1}^{N} s_i \\ \text{s.t.} & \frac{\lambda}{N} c(\xi, \widehat{\xi}_i) + s_i \geq \frac{1}{N} I(\xi) \quad \forall \xi \in \Xi \end{array} \right.$$

$$= \inf_{\lambda\geq 0} \ \lambda\varepsilon + \frac{1}{N}\sum_{i=1}^{N} \sup_{\xi\in\Xi} \ I(\xi) - \lambda c(\xi, \widehat{\xi}_i)$$

$$= \inf_{\lambda\geq 0} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{\zeta\in\Xi} I(\zeta) - \lambda c(\zeta, \xi)\right]$$

Proof of Lemma 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[I(\xi)\right] \overset{\text{[S01]}}{\boxed{\leq}} \left\{ \begin{array}{ll} \inf\limits_{\substack{\lambda\geq 0 \\ s\in\mathbb{R}^N}} & \lambda\varepsilon + \sum\limits_{i=1}^{N} s_i \\ \\ \text{s.t.} & \dfrac{\lambda}{N} c(\xi, \widehat{\xi}_i) + s_i \geq \dfrac{1}{N} I(\xi) \quad \forall \xi \in \Xi \end{array} \right.$$

$$= \inf_{\lambda\geq 0} \; \lambda\varepsilon + \frac{1}{N}\sum_{i=1}^{N} \sup_{\xi\in\Xi} \; I(\xi) - \lambda c(\xi, \widehat{\xi}_i)$$

$$= \inf_{\lambda\geq 0} \; \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{\zeta\in\Xi} I(\zeta) - \lambda c(\zeta, \xi)\right]$$

Semi-infinite Duality

Lemma 1. Let $\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\Xi) : W_c(\mathbb{Q}, \widehat{\mathbb{P}}_N) \leq \varepsilon\}$. If $c(\xi, \xi) = 0$ for all $\xi \in \Xi$ and $\varepsilon > 0$, then

$$\sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}}[I(\xi)] = \inf_{\lambda \geq 0} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{\zeta \in \Xi} I(\zeta) - \lambda c(\zeta, \xi)\right]$$

[MK18, ZG18, BM19, GK16, ZYG22]

Lipschitz Envelope

Lemma 2. Let $L : \mathbb{R} \to \mathbb{R}$ be a convex and Lipschitz function. Then,

$$\sup_{\zeta \in \mathbb{R}^n} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| = \begin{cases} L(\theta^\top \xi + \theta_0) & \text{if } \; \mathrm{lip(L)} \|\theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

for any $\theta, \xi \in \mathbb{R}^n, \theta_0 \in \mathbb{R}$ and $\lambda > 0$.

[SKM19]

Proof of Lemma 2

$$L(\theta^\top \zeta + \theta_0) = L^{**}(\theta^\top \zeta + \theta_0) = \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa)$$

$$\mathcal{K} = \{\kappa \in \mathbb{R} : L^*(\kappa) < \infty\}$$

Proof of Lemma 2

$$L(\theta^\top \zeta + \theta_0) = L^{**}(\theta^\top \zeta + \theta_0) = \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa)$$

$$\mathcal{K} = \{\kappa \in \mathbb{R} : L^*(\kappa) < \infty\}$$

$$\sup_{\zeta} \ L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| = \sup_{\zeta} \ \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - \lambda \|\zeta - \xi\|$$

Proof of Lemma 2

$$L(\theta^\top \zeta + \theta_0) = L^{**}(\theta^\top \zeta + \theta_0) = \sup_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa)$$

$$\mathcal{K} = \{\kappa \in \mathbb{R} : L^*(\kappa) < \infty\}$$

$$\boxed{\sup_{\|p\|_* \le \lambda} \; p^\top(\zeta - \xi)}$$

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda\|\zeta - \xi\| = \sup_{\zeta} \; \sup_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - \boxed{\lambda\|\zeta - \xi\|}$$

$$= \sup_{\kappa \in \mathcal{K}} \; \sup_{\zeta} \; \inf_{\|p\|_* \le \lambda} \; \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - p^\top(\zeta - \xi)$$

Proof of Lemma 2

$$L(\theta^\top \zeta + \theta_0) = L^{**}(\theta^\top \zeta + \theta_0) = \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa)$$

$$\mathcal{K} = \{\kappa \in \mathbb{R} : L^*(\kappa) < \infty\}$$

$$\begin{aligned}
\sup_{\zeta} \ L(\theta^\top \zeta + \theta_0) - \lambda\|\zeta - \xi\| &= \sup_{\zeta} \ \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - \lambda\|\zeta - \xi\| \\
&= \sup_{\kappa \in \mathcal{K}} \ \sup_{\zeta} \ \inf_{\|p\|_* \le \lambda} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - p^\top(\zeta - \xi) \\
\textbf{(Sion's minimax)} \quad &= \sup_{\kappa \in \mathcal{K}} \ \inf_{\|p\|_* \le \lambda} \ \sup_{\zeta} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - p^\top(\zeta - \xi)
\end{aligned}$$

Proof of Lemma 2

$$L(\theta^\top \zeta + \theta_0) = L^{**}(\theta^\top \zeta + \theta_0) = \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa)$$

$$\mathcal{K} = \{\kappa \in \mathbb{R} : L^*(\kappa) < \infty\}$$

$$\begin{aligned}
\sup_{\zeta} \ L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| &= \sup_{\zeta} \ \sup_{\kappa \in \mathcal{K}} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - \lambda \|\zeta - \xi\| \\
&= \sup_{\kappa \in \mathcal{K}} \ \sup_{\zeta} \ \inf_{\|p\|_* \le \lambda} \ \kappa(\theta^\top \zeta + \theta_0) - L^*(\kappa) - p^\top(\zeta - \xi) \\
\textbf{(Sion's minimax)} \quad &= \sup_{\kappa \in \mathcal{K}} \ \inf_{\|p\|_* \le \lambda} \ \kappa\theta_0 - L^*(\kappa) + p^\top \xi + \begin{cases} 0 & \text{if } \kappa\theta - p = 0 \\ +\infty & \text{else} \end{cases}
\end{aligned}$$

Proof of Lemma 2

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| = \sup_{\kappa \in \mathcal{K}} \; \begin{cases} \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa\theta\|_* \leq \lambda \\ \\ +\infty & \text{else} \end{cases}$$

Proof of Lemma 2

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| = \sup_{\kappa \in \mathcal{K}} \begin{cases} \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa \theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

$$= \begin{cases} \sup_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa \theta\|_* \leq \lambda \; \forall \kappa \in \mathcal{K} \\ +\infty & \text{else} \end{cases}$$

Proof of Lemma 2

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| = \sup_{\kappa \in \mathcal{K}} \begin{cases} \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa\theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

$$= \begin{cases} \sup_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa\theta\|_* \leq \lambda \; \forall \kappa \in \mathcal{K} \\ +\infty & \text{else} \end{cases}$$

$$= \begin{cases} \sup_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \sup_{\kappa \in \mathcal{K}} \|\kappa\theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

Proof of Lemma 2

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\| = \sup_{\kappa \in \mathcal{K}} \begin{cases} \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa\theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

$$= \begin{cases} \sup\limits_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \|\kappa\theta\|_* \leq \lambda \; \forall \kappa \in \mathcal{K} \\ +\infty & \text{else} \end{cases}$$

$$= \begin{cases} \sup\limits_{\kappa \in \mathcal{K}} \; \kappa(\theta^\top \xi + \theta_0) - L^*(\kappa) & \text{if } \sup\limits_{\kappa \in \mathcal{K}} \|\kappa\theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

$$\boxed{\sup_{\kappa \in \mathcal{K}} |\kappa| = \text{lip}(L)} = \begin{cases} L(\theta^\top \xi + \theta_0) & \text{if } \text{lip}(L)\|\theta\|_* \leq \lambda \\ +\infty & \text{else} \end{cases}$$

Tractability for Linear Regression

Theorem 1. Suppose that $c\big((x,y),(x',y')\big) = \|x-x'\| + \delta_{y=y'}$.

If L is convex and Lipschitz, then

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right] = \inf_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} L(\theta^\top \widehat{x}_i - \widehat{y}_i) + \varepsilon \mathrm{lip}(L)\|\theta\|_*$$

[SMK15, GCK17, SKM19, BKM19]

Proof of Theorem 1

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x', y') \in \mathbb{R}^n \times \mathbb{R}} L(\theta^\top x' - y') - \lambda \|x' - x\| - \lambda \delta_{y' = y} \right]$$

Proof of Theorem 1

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \ \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \ \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x', y') \in \mathbb{R}^n \times \mathbb{R}} L(\theta^\top x' - y') - \lambda \|x' - x\| - \lambda \delta_{y' = y} \right]$$

$$= \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \ \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{x' \in \mathbb{R}^n} L(\theta^\top x' - y) - \lambda \|x' - x\| \right]$$

Proof of Theorem 1

$$\inf_{\theta\in\Theta}\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(\theta^\top x' - y') - \lambda\|x'-x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(\theta^\top x' - y) - \lambda\|x'-x\|\right]$$

$$\textbf{(Lemma 2)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\begin{cases} L(\theta^\top x - y) & \text{if } \lambda \geq \operatorname{lip}(L)\|\theta\|_* \\ +\infty & \text{else}\end{cases}\right]$$

Proof of Theorem 1

$$\inf_{\theta\in\Theta}\sup_{\mathbb{Q}\in\mathcal{P}}\ \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(\theta^\top x' - y') - \lambda\|x' - x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(\theta^\top x' - y) - \lambda\|x' - x\|\right]$$

$$\textbf{(Lemma 2)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq \mathrm{lip}(L)\|\theta\|_*}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(\theta^\top x - y)\right]$$

Proof of Theorem 1

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(\theta^\top x' - y') - \lambda\|x' - x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(\theta^\top x' - y) - \lambda\|x' - x\|\right]$$

$$\textbf{(Lemma 2)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq \mathrm{lip}(L)\|\theta\|_*}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(\theta^\top x - y)\right]$$

$$= \inf_{\theta\in\Theta} \varepsilon\,\mathrm{lip}(L)\|\theta\|_* + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(\theta^\top x - y)\right]$$

Examples

Robust Regression

$$L(z) = \begin{cases} \frac{1}{2} z^2 & \text{if } \ |z| \leq \delta \\ \delta \left(|z| - \frac{1}{2}\delta \right) & \text{else} \end{cases}$$

$$\operatorname{lip}(L) = \delta$$

✓

Support Vector Regression

$$L(z) = \max\{0, |z| - \varepsilon\}$$

$$\operatorname{lip}(L) = 1$$

✓

Quantile Regression

$$L(z) = \max\{-\tau z, (1-\tau)z\}$$

$$\operatorname{lip}(L) = \max\{\tau, 1-\tau\}$$

✓

Examples

Least Square Regression

$$L(z) = z^2$$

$$\mathrm{lip}(L) = \infty$$

✗

Least Squares Regression

Theorem 2. Suppose that $c\big((x,y),(x',y')\big) = \|x - x'\|^2 + \delta_{y=y'}$.

If $L = z^2$, then

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right] = \left(\inf_{\theta \in \Theta} \sqrt{\frac{1}{N} \sum_{i=1}^{N} L(\widehat{y}_i \theta^\top \widehat{x}_i)} + \sqrt{\varepsilon} \|\theta\|_* \right)^2$$

[BKM19]

Moreau Envelope

Lemma 3. Let $L(z) = z^2$. Then,

$$\sup_{\zeta \in \mathbb{R}^n} L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 = \begin{cases} \dfrac{\lambda}{\lambda - \|\theta\|_*^2} L(\theta^\top \xi + \theta_0) & \text{if } \|\theta\|_*^2 < \lambda \\ +\infty & \text{else} \end{cases}$$

for any $\theta, \xi \in \mathbb{R}^n, \theta_0 \in \mathbb{R}$ and $\lambda > 0$.

[BKM19, SADK22]

Proof of Lemma 3

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda\|\zeta - \xi\|^2$$

$$\boxed{\Delta \leftarrow \zeta - \xi} \quad = \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2$$

Proof of Lemma 3

$$
\begin{aligned}
&\sup_{\zeta}\ L(\theta^\top \zeta + \theta_0) - \lambda\|\zeta - \xi\|^2 \\
&= \sup_{\Delta}\ L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 \\
&= \left\{ \begin{array}{ll} \sup\limits_{\Delta,\gamma} & L(\gamma + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right.
\end{aligned}
$$

Proof of Lemma 3

$$
\begin{aligned}
&\sup_{\zeta}\; L(\theta^\top \zeta + \theta_0) - \lambda\|\zeta - \xi\|^2 \\
&= \sup_{\Delta}\; L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 \\
&= \sup_{\gamma} \left\{ \begin{array}{ll} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right.
\end{aligned}
$$

Proof of Lemma 3

$$
\begin{aligned}
& \sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 \\
&= \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 \\
&= \sup_{\gamma} \begin{cases} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{cases} \\
\textbf{(Slater condition)} &= \sup_{\gamma} \; \inf_{\kappa} \; \sup_{\Delta} \; L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 - \kappa\gamma + \kappa\theta^\top \Delta
\end{aligned}
$$

Proof of Lemma 3

$$
\begin{aligned}
& \sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 \\
&= \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 \\
&= \sup_{\gamma} \begin{cases} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{cases} \\
\textbf{(Slater condition)} &= \sup_{\gamma} \; \inf_{\kappa} \; \sup_{\Delta} \; L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 - \kappa\gamma + \kappa\theta^\top \Delta \\
\textbf{(Holder inequality)} &\leq \sup_{\gamma} \; \inf_{\kappa} \; \sup_{\Delta} \; L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 - \kappa\gamma + \|\kappa\theta\|_* \|\Delta\|
\end{aligned}
$$

Proof of Lemma 3

$$
\begin{aligned}
& \sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 \\
& = \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 \\
& = \sup_{\gamma} \begin{cases} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{cases} \\
\textbf{(Slater condition)} & = \sup_{\gamma} \; \inf_{\kappa} \; \sup_{\Delta} \; L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 - \kappa\gamma + \kappa\theta^\top \Delta \\
\textbf{(Holder inequality)} & = \sup_{\gamma} \; \inf_{\kappa} \; \sup_{\|\Delta\|} \; L(\gamma + \theta^\top \xi + \theta_0) - \lambda \|\Delta\|^2 - \kappa\gamma + \|\kappa\theta\|_* \|\Delta\|
\end{aligned}
$$

$$\boxed{\|\Delta^\star\| = \frac{\|\kappa\theta\|_*}{2\lambda}}$$

Proof of Lemma 3

$$
\begin{aligned}
&\sup_{\zeta}\ L(\theta^\top \zeta + \theta_0) - \lambda\|\zeta - \xi\|^2 \\
&= \sup_{\Delta}\ L(\theta^\top \Delta + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 \\
&= \sup_{\gamma} \left\{ \begin{array}{ll} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right. \\
\textbf{(Slater condition)} \ &= \sup_{\gamma}\ \inf_{\kappa}\ \sup_{\Delta}\ L(\gamma + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 - \kappa\gamma + \kappa\theta^\top \Delta \\
\textbf{(Holder inequality)} &= \sup_{\gamma}\ \inf_{\kappa}\ \sup_{\|\Delta\|}\ L(\gamma + \theta^\top \xi + \theta_0) - \lambda\|\Delta\|^2 - \kappa\gamma + \|\kappa\theta\|_*\|\Delta\| \\
&= \sup_{\gamma}\ \inf_{\kappa}\ L(\gamma + \theta^\top \xi + \theta_0) - \kappa\gamma + \frac{\|\kappa\theta\|_*^2}{4\lambda} \qquad \boxed{\kappa^\star = \frac{2\lambda\gamma}{\|\theta\|_*^2}}
\end{aligned}
$$

Proof of Lemma 3

$$\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 = \sup_{\gamma} \; L(\gamma + \theta^\top \xi) - \frac{\lambda \gamma^2}{\|\theta\|_*^2}$$

Proof of Lemma 3

$$
\begin{aligned}
\sup_{\zeta} \; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 &= \sup_{\gamma} \; L(\gamma + \theta^\top \xi) - \frac{\lambda \gamma^2}{\|\theta\|_*^2} \\
&= \sup_{\gamma} \; (\gamma + \theta^\top \xi)^2 - \frac{\lambda \gamma^2}{\|\theta\|_*^2}
\end{aligned}
$$

$$
\boxed{\begin{cases} \gamma^\star = \frac{\theta^\top \xi}{\frac{\lambda}{\|\theta\|_*^2} - 1} & \text{if } 1 - \frac{\lambda}{\|\theta\|_*^2} < 0 \\ \text{unbounded} & \text{else} \end{cases}}
$$

Proof of Lemma 3

$$
\begin{aligned}
\sup_{\zeta}\; L(\theta^\top \zeta + \theta_0) - \lambda \|\zeta - \xi\|^2 &= \sup_{\gamma}\; L(\gamma + \theta^\top \xi) - \frac{\lambda \gamma^2}{\|\theta\|_*^2} \\
&= \sup_{\gamma}\; (\gamma + \theta^\top \xi)^2 - \frac{\lambda \gamma^2}{\|\theta\|_*^2} \\
&= \begin{cases} \dfrac{\lambda}{\lambda - \|\theta\|_*^2} (\theta^\top \xi)^2 & \text{if } \|\theta\|_*^2 < \lambda \\ +\infty & \text{else} \end{cases}
\end{aligned}
$$

Least Squares Regression

Theorem 2. Suppose that $c\big((x,y),(x',y')\big) = \|x-x'\|^2 + \delta_{y=y'}$.

If $L = z^2$, then

$$\inf_{\theta\in\Theta}\ \sup_{\mathbb{Q}\in\mathcal{P}}\ \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right] = \inf_{\theta\in\Theta}\ \left(\sqrt{\frac{1}{N}\sum_{i=1}^{N} L(\theta^\top \widehat{x}_i - \widehat{y}_i)} + \sqrt{\varepsilon}\|\theta\|_*\right)^2$$

[BKM19]

Proof of Theorem 2

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x', y') \in \mathbb{R}^n \times \mathbb{R}} L(\theta^\top x' - y') - \lambda \|x' - x\|^2 - \lambda \delta_{y' = y} \right]$$

Proof of Theorem 2

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \; \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \; \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x', y') \in \mathbb{R}^n \times \mathbb{R}} L(\theta^\top x' - y') - \lambda \|x' - x\|^2 - \lambda \delta_{y' = y} \right]$$

$$= \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \; \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{x' \in \mathbb{R}^n} L(\theta^\top x' - y) - \lambda \|x' - x\|^2 \right]$$

Proof of Theorem 2

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(\theta^\top x - y) \right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x', y') \in \mathbb{R}^n \times \mathbb{R}} L(\theta^\top x' - y') - \lambda \|x' - x\|^2 - \lambda \delta_{y' = y} \right]$$

$$= \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{x' \in \mathbb{R}^n} L(\theta^\top x' - y) - \lambda \|x' - x\|^2 \right]$$

$$\textbf{(Lemma 3)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\begin{cases} \frac{\lambda}{\lambda - \|\theta\|_*^2} L(\theta^\top x - y) & \text{if } \lambda > \|\theta\|_*^2 \\ +\infty & \text{else} \end{cases} \right]$$

Proof of Theorem 2

$$\inf_{\theta\in\Theta}\ \sup_{\mathbb{Q}\in\mathcal{P}}\ \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right]$$

(Lemma 1) $$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(\theta^\top x' - y') - \lambda\|x' - x\|^2 - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(\theta^\top x' - y) - \lambda\|x' - x\|^2\right]$$

(Lemma 3) $$= \inf_{\substack{\theta\in\Theta\\ \lambda>\|\theta\|_*^2}}\ \lambda\varepsilon + \frac{\lambda}{\lambda - \|\theta\|_*^2}\mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(\theta^\top x - y)\right]$$

$$\boxed{\lambda^\star = \|\theta\|_*^2 + \frac{\|\theta\|_*\sqrt{\mathbb{E}_{\widehat{\mathbb{P}}_N}[L(\theta^\top x - y)]}}{\varepsilon}}$$

Proof of Theorem 2

$$\inf_{\theta\in\Theta}\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(\theta^\top x - y)\right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(\theta^\top x' - y') - \lambda\|x'-x\|^2 - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(\theta^\top x' - y) - \lambda\|x'-x\|^2\right]$$

$$\textbf{(Lemma 3)} = \inf_{\substack{\theta\in\Theta\\ \lambda>\|\theta\|_*^2}} \lambda\varepsilon + \frac{\lambda}{\lambda-\|\theta\|_*^2}\mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(\theta^\top x - y)\right]$$

$$= \inf_{\theta\in\Theta} \left(\sqrt{\varepsilon}\|\theta\|_* + \sqrt{\mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(\theta^\top x - y)\right]}\right)^2$$

Tractability for Linear Classification

Theorem 3. Suppose that $c\big((x,y),(x',y')\big) = \|x - x'\| + \delta_{y=y'}$.

If L is convex and Lipschitz, then

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right] = \inf_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} L(\widehat{y}_i\theta^\top\widehat{x}_i) + \varepsilon \mathrm{lip}(L)\|\theta\|_*$$

[SMK15, GCK17, SKM19, BKM19]

Proof of Theorem 3

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \ \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

$$\textbf{(Lemma 1)} \ = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(y'\theta^\top x') - \lambda\|x'-x\| - \lambda\delta_{y'=y}\right]$$

Proof of Theorem 3

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(y \theta^\top x) \right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x', y') \in \mathbb{R}^n \times \mathbb{R}} L(y' \theta^\top x') - \lambda \| x' - x \| - \lambda \delta_{y' = y} \right]$$

$$= \inf_{\substack{\theta \in \Theta \\ \lambda \geq 0}} \lambda \varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{x' \in \mathbb{R}^n} L(y \theta^\top x') - \lambda \| x' - x \| \right]$$

Proof of Theorem 3

$$\inf_{\theta\in\Theta}\ \sup_{\mathbb{Q}\in\mathcal{P}}\ \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

$$\textbf{(Lemma 1)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(y'\theta^\top x') - \lambda\|x'-x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(y\theta^\top x') - \lambda\|x'-x\|\right]$$

$$\textbf{(Lemma 2)} = \inf_{\substack{\theta\in\Theta\\ \lambda\geq \mathrm{lip}(L)\|\theta\|_*}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(y\theta^\top x)\right]$$

Proof of Theorem 3

$$\inf_{\theta\in\Theta}\ \sup_{\mathbb{Q}\in\mathcal{P}}\ \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

$$\textbf{(Lemma 1)}\ = \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(y'\theta^\top x') - \lambda\|x'-x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta\in\Theta\\ \lambda\geq 0}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(y\theta^\top x') - \lambda\|x'-x\|\right]$$

$$\textbf{(Lemma 2)}\ = \inf_{\substack{\theta\in\Theta\\ \lambda\geq \mathrm{lip}(L)\|\theta\|_*}}\ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(y\theta^\top x)\right]$$

$$= \inf_{\theta\in\Theta}\ \varepsilon\,\mathrm{lip}(L)\|\theta\|_* + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L(y\theta^\top x)\right]$$

Examples

Support Vector Machine

$$L(z) = \max\{0, 1 - z\}$$

$$\mathrm{lip}(L) = 1$$

✓

Support Vector Machine II

$$L(z) = \begin{cases} \frac{1}{2} - z & \text{if } z \leq 0 \\ \frac{1}{2}(1-z)^2 & \text{if } 0 < z < 1 \\ 0 & \text{else} \end{cases}$$

$$\mathrm{lip}(L) = 1$$

✓

Logistic Regression

$$L(z) = \log(1 + \exp(-z))$$

$$\mathrm{lip}(L) = 1$$

✓

Examples

Ideal Classification

$$L(z) = \begin{cases} 1 & \text{if } z \leq 0 \\ 0 & \text{else} \end{cases}$$

nonconvex!

✗

Ideal Classification

Theorem 4. Suppose that $c\big((x,y),(x',y')\big) = \|x - x'\| + \delta_{y=y'}$.

If $L(z) = \mathbb{1}_{z\leq 0}$, then

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right] = \inf_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} L_R(\widehat{y}_i\theta^\top\widehat{x}_i) + \varepsilon\|\theta\|_*$$

where $L_R(z) = \max\{0, 1-z\} + \max\{0, -z\}$.

[H-NW22]

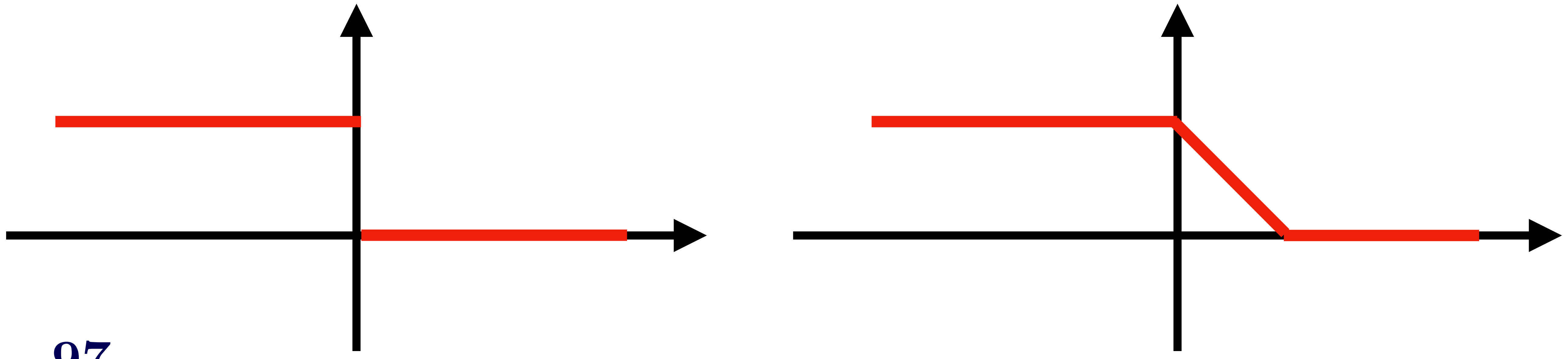
Ideal Classification

Theorem 4. Suppose that $c\big((x,y),(x',y')\big) = \|x - x'\| + \delta_{y=y'}$.

If $L(z) = \mathbb{1}_{z\leq 0}$, then

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right] = \inf_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} L_R(\widehat{y}_i\theta^\top\widehat{x}_i) + \varepsilon\|\theta\|_*$$

where $L_R(z) = \max\{0, 1 - z\} + \max\{0, -z\}$.



[H-NW22]

Lipschitz Envelope II

Lemma 4. Let $L(z) = \mathbb{1}_{z \le 0}$. Then,

$$\sup_{\zeta \in \mathbb{R}^n} L(\theta^\top \zeta) - \lambda \|\zeta - \xi\| = L_R\big(\lambda(\theta^\top \xi)/\|\theta\|_*\big)$$

for any $\theta, \xi \in \mathbb{R}^n$ and $\lambda > 0$.

[SADK22]

Proof of Lemma 4

$$\sup_{\zeta} \ L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| = \sup_{\Delta} \ L(\theta^\top \Delta + \theta^\top \xi) - \lambda\|\Delta\|$$

$\boxed{\Delta \leftarrow \zeta - \xi}$

Proof of Lemma 4

$$\sup_{\zeta} \; L(\theta^\top \zeta) - \lambda \|\zeta - \xi\| = \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi) - \lambda \|\Delta\|$$

$$= \left\{ \begin{array}{ll} \sup\limits_{\Delta,\gamma} & L(\gamma + \theta^\top \xi) - \lambda \|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right.$$

Proof of Lemma 4

$$\sup_{\zeta} \; L(\theta^\top \zeta) - \lambda \|\zeta - \xi\| = \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi) - \lambda \|\Delta\|$$

$$= \sup_{\gamma} \left\{ \begin{array}{ll} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi) - \lambda \|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right.$$

Proof of Lemma 4

$$\sup_{\zeta} \; L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| = \sup_{\Delta} \; L(\theta^\top \Delta + \theta^\top \xi) - \lambda\|\Delta\|$$

$$= \sup_{\gamma} \begin{cases} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{cases}$$

$$\textbf{(Slater condition)} = \sup_{\gamma} \; \inf_{\kappa} \; \sup_{\Delta} \; L(\gamma + \theta^\top \xi) - \boxed{\lambda\|\Delta\|} - \kappa\gamma + \kappa\theta^\top \Delta$$

Proof of Lemma 4

$$
\begin{aligned}
\sup_{\zeta}\; L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| &= \sup_{\Delta}\; L(\theta^\top \Delta + \theta^\top \xi) - \lambda\|\Delta\| \\
&= \sup_{\gamma} \left\{ \begin{array}{ll} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right. \\
\textbf{(Slater condition)} &= \sup_{\gamma}\; \inf_{\kappa}\; \sup_{\Delta}\; L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| - \kappa\gamma + \kappa\theta^\top \Delta \\
&= \sup_{\gamma}\; \inf_{\kappa}\; \sup_{\Delta}\; \inf_{\|p\|_* \le \lambda}\; L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta
\end{aligned}
$$

Proof of Lemma 4

$$\begin{aligned}
\sup_{\zeta}\ L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| &= \sup_{\Delta}\ L(\theta^\top \Delta + \theta^\top \xi) - \lambda\|\Delta\| \\
&= \sup_{\gamma} \left\{ \begin{array}{ll} \sup\limits_{\Delta} & L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right. \\
\textbf{(Slater condition)} &= \sup_{\gamma}\ \inf_{\kappa}\ \sup_{\Delta}\ L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| - \kappa\gamma + \kappa\theta^\top \Delta \\
&= \sup_{\gamma}\ \inf_{\kappa}\ \sup_{\Delta}\ \inf_{\|p\|_* \le \lambda}\ L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta \\
\textbf{(Sion's minimax)} &= \sup_{\gamma}\ \inf_{\substack{\kappa \\ \|p\|_* \le \lambda}}\ \sup_{\Delta}\ L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta
\end{aligned}$$

Proof of Lemma 4

$$\sup_{\zeta} L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| = \sup_{\Delta} L(\theta^\top \Delta + \theta^\top \xi) - \lambda\|\Delta\|$$

$$= \sup_{\gamma} \begin{cases} \sup_{\Delta} & L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{cases}$$

$$\textbf{(Slater condition)} = \sup_{\gamma} \inf_{\kappa} \sup_{\Delta} L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| - \kappa\gamma + \kappa\theta^\top \Delta$$

$$= \sup_{\gamma} \inf_{\kappa} \sup_{\Delta} \inf_{\|p\|_* \leq \lambda} L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta$$

$$\textbf{(Sion's minimax)} = \sup_{\gamma} \inf_{\substack{\kappa \\ \|p\|_* \leq \lambda}} \sup_{\Delta} L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta$$

$$= \sup_{\gamma} \inf_{\substack{\kappa \\ \|p\|_* \leq \lambda}} L(\gamma + \theta^\top \xi) - \kappa\gamma + \begin{cases} 0 & \text{if } \kappa\theta - p = 0 \\ +\infty & \text{else} \end{cases}$$

Proof of Lemma 4

$$
\begin{aligned}
\sup_{\zeta}\; L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| &= \sup_{\Delta}\; L(\theta^\top \Delta + \theta^\top \xi) - \lambda\|\Delta\| \\
&= \sup_{\gamma} \left\{ \begin{array}{ll} \displaystyle\sup_{\Delta} & L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| \\ \text{s.t.} & \gamma = \theta^\top \Delta \end{array} \right. \\
\textbf{(Slater condition)} &= \sup_{\gamma}\; \inf_{\kappa}\; \sup_{\Delta}\; L(\gamma + \theta^\top \xi) - \lambda\|\Delta\| - \kappa\gamma + \kappa\theta^\top \Delta \\
&= \sup_{\gamma}\; \inf_{\kappa}\; \sup_{\Delta}\; \inf_{\|p\|_* \le \lambda}\; L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta \\
\textbf{(Sion's minimax)} &= \sup_{\gamma}\; \inf_{\substack{\kappa \\ \|p\|_* \le \lambda}}\; \sup_{\Delta}\; L(\gamma + \theta^\top \xi) - p^\top \Delta - \kappa\gamma + \kappa\theta^\top \Delta \\
&= \sup_{\gamma}\; \inf_{-\lambda/\|\theta\|_* \le \kappa \le \lambda/\|\theta\|_*}\; L(\gamma + \theta^\top \xi) - \kappa\gamma \quad \boxed{\kappa^\star = \frac{\lambda}{\|\theta\|_*}\operatorname{sgn}(\gamma)}
\end{aligned}
$$

Proof of Lemma 4

$$\sup_{\zeta}\ L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| = \sup_{\gamma}\ L(\gamma + \theta^\top \xi) - \frac{\lambda|\gamma|}{\|\theta\|_*}$$

Proof of Lemma 4

$$\begin{aligned}
\sup_{\zeta} \; L(\theta^\top \zeta) - \lambda \|\zeta - \xi\| &= \sup_{\gamma} \; L(\gamma + \theta^\top \xi) - \frac{\lambda |\gamma|}{\|\theta\|_*} \\
&= \sup_{\gamma} \; L(\gamma \|\theta\|_* + \theta^\top \xi) - \lambda |\gamma| \qquad \boxed{\gamma \leftarrow \gamma / \|\theta\|_*}
\end{aligned}$$

Proof of Lemma 4

$$\begin{aligned}
\sup_{\zeta}\ L(\theta^\top \zeta) - \lambda \|\zeta - \xi\| &= \sup_{\gamma}\ L(\gamma + \theta^\top \xi) - \frac{\lambda|\gamma|}{\|\theta\|_*} \\
&= \sup_{\gamma}\ L(\gamma\|\theta\|_* + \theta^\top \xi) - \lambda|\gamma| \\
&= \sup_{\gamma}\ \begin{cases} 1 - \lambda|\gamma| & \text{if } \gamma\|\theta\|_* + \theta^\top \xi \le 0 \\ -\lambda|\gamma| & \text{else} \end{cases}
\end{aligned}$$

Proof of Lemma 4

$$\begin{aligned}
\sup_{\zeta}\ L(\theta^\top \zeta) - \lambda\|\zeta - \xi\| &= \sup_{\gamma}\ L(\gamma + \theta^\top \xi) - \frac{\lambda|\gamma|}{\|\theta\|_*} \\
&= \sup_{\gamma}\ L(\gamma\|\theta\|_* + \theta^\top \xi) - \lambda|\gamma| \\
&= \sup_{\gamma}\ \begin{cases} 1 - \lambda|\gamma| & \text{if } \gamma\|\theta\|_* + \theta^\top \xi \leq 0 \\ -\lambda|\gamma| & \text{else} \end{cases} \\
&= \begin{cases} 1 & \text{if } \theta^\top \xi \leq 0 \\ \max\{0, 1 - \lambda\frac{\theta^\top \xi}{\|\theta\|_*}\} & \text{else} \end{cases}
\end{aligned}$$

Proof of Lemma 4

$$\begin{aligned}
\sup_{\zeta}\ L(\theta^\top\zeta) - \lambda\|\zeta - \xi\| &= \sup_{\gamma}\ L(\gamma + \theta^\top\xi) - \frac{\lambda|\gamma|}{\|\theta\|_*} \\
&= \sup_{\gamma}\ L(\gamma\|\theta\|_* + \theta^\top\xi) - \lambda|\gamma| \\
&= \sup_{\gamma}\ \begin{cases} 1 - \lambda|\gamma| & \text{if } \gamma\|\theta\|_* + \theta^\top\xi \le 0 \\ -\lambda|\gamma| & \text{else} \end{cases} \\
&= \begin{cases} 1 & \text{if } \theta^\top\xi \le 0 \\ \max\{0, 1 - \lambda\frac{\theta^\top\xi}{\|\theta\|_*}\} & \text{else} \end{cases} \\
&= L_R\big(\lambda(\theta^\top\xi)/\|\theta\|_*\big)
\end{aligned}$$

Ideal Classification

Theorem 4. Suppose that $c\big((x,y),(x',y')\big) = \|x - x'\| + \delta_{y=y'}$.

If $L(z) = \mathbb{1}_{z\leq 0}$, then

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right] = \inf_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} L_R(\widehat{y}_i\theta^\top\widehat{x}_i) + \varepsilon\|\theta\|_*$$

where $L_R(z) = \max\{0, 1 - z\} + \max\{0, -z\}$.

[H-NW22]

Proof of Theorem 4

$$\inf_{\theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

$$\textbf{(Lemma 1)} \quad = \inf_{\substack{\theta \\ \lambda \geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y') \in \mathbb{R}^n \times \mathbb{R}} L(y'\theta^\top x') - \lambda\|x' - x\| - \lambda\delta_{y'=y}\right]$$

Proof of Theorem 4

$$\inf_{\theta} \sup_{\mathbb{Q}\in\mathcal{P}} \; \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

$$\textbf{(Lemma 1)} \; = \inf_{\substack{\theta \\ \lambda\geq 0}} \; \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(y'\theta^\top x') - \lambda\|x' - x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta \\ \lambda\geq 0}} \; \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(y\theta^\top x') - \lambda\|x' - x\|\right]$$

Proof of Theorem 4

$$\inf_{\theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[L(y\theta^\top x) \right]$$

$$\textbf{(Lemma 1)} \quad = \inf_{\substack{\theta \\ \lambda \geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{(x',y') \in \mathbb{R}^n \times \mathbb{R}} L(y'\theta^\top x') - \lambda\|x' - x\| - \lambda\delta_{y'=y} \right]$$

$$= \inf_{\substack{\theta \\ \lambda \geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[\sup_{x' \in \mathbb{R}^n} L(y\theta^\top x') - \lambda\|x' - x\| \right]$$

$$\textbf{(Lemma 4)} \quad = \inf_{\substack{\theta \\ \lambda \geq 0}} \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N} \left[L_R\big(\lambda(y\theta^\top x)/\|\theta\|_*\big) \right]$$

Proof of Theorem 4

$$\inf_{\theta} \sup_{\mathbb{Q}\in\mathcal{P}} \ \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

(Lemma 1) $$= \inf_{\substack{\theta \\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(y'\theta^\top x') - \lambda\|x'-x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta \\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(y\theta^\top x') - \lambda\|x'-x\|\right]$$

(Lemma 4) $$= \inf_{\substack{\theta \\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L_R\big(\lambda(y\theta^\top x)/\|\theta\|_*\big)\right]$$

$$\boxed{\begin{array}{c} \theta \leftarrow \lambda\theta/\|\theta\|_* \\ \Downarrow \\ \lambda = \|\theta\|_* \end{array}}$$

Proof of Theorem 4

$$\inf_{\theta} \sup_{\mathbb{Q}\in\mathcal{P}} \ \mathbb{E}_{\mathbb{Q}}\left[L(y\theta^\top x)\right]$$

$$\textbf{(Lemma 1)} \quad = \inf_{\substack{\theta \\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{(x',y')\in\mathbb{R}^n\times\mathbb{R}} L(y'\theta^\top x') - \lambda\|x'-x\| - \lambda\delta_{y'=y}\right]$$

$$= \inf_{\substack{\theta \\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[\sup_{x'\in\mathbb{R}^n} L(y\theta^\top x') - \lambda\|x'-x\|\right]$$

$$\textbf{(Lemma 4)} \quad = \inf_{\substack{\theta \\ \lambda\geq 0}} \ \lambda\varepsilon + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L_R\big(\lambda(y\theta^\top x)/\|\theta\|_*\big)\right]$$

$$= \inf_{\theta} \ \varepsilon\|\theta\|_* + \mathbb{E}_{\widehat{\mathbb{P}}_N}\left[L_R(y\theta^\top x)\right]$$

$$\boxed{\begin{array}{c} \theta \leftarrow \lambda\theta/\|\theta\|_* \\ \Downarrow \\ \lambda = \|\theta\|_* \end{array}}$$

Conclusion

Regularization = Distributional Robustness

Take Away

$$\inf_{\theta \in \boldsymbol{\Theta}} \sup_{\mathbb{Q} \in \mathcal{P}} \; \mathbb{E}_{\mathbb{Q}} \left[\ell(\theta, \xi) \right]$$

$$\mathcal{P} = \{ \mathbb{Q} \in \mathcal{M}(\Xi) : W_c(\mathbb{Q}, \mathbb{P}) \leq \varepsilon \}$$

Take Away

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\ell(\theta, \xi) \right]$$

$$\mathcal{P} = \{ \mathbb{Q} \in \mathcal{M}(\Xi) : W_c(\mathbb{Q}, \mathbb{P}) \leq \varepsilon \}$$

Step 1

$$\sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\ell(\theta, \xi) \right] = \inf_{\lambda \geq 0} \lambda \varepsilon + \mathbb{E}_{\mathbb{P}} \left[\sup_{\zeta \in \Xi} \ell(\theta, \zeta) - \lambda c(\zeta, \xi) \right]$$

[MK18, ZG18, BM19, GK16, ZYG22]

Take Away

$$\inf_{\theta \in \Theta} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\ell(\theta, \xi) \right]$$

$$\mathcal{P} = \{ \mathbb{Q} \in \mathcal{M}(\Xi) : W_c(\mathbb{Q}, \mathbb{P}) \leq \varepsilon \}$$

Step 1

$$\sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\ell(\theta, \xi) \right] = \inf_{\lambda \geq 0} \lambda \varepsilon + \mathbb{E}_{\mathbb{P}} \left[\boxed{\sup_{\zeta \in \Xi} \ell(\theta, \zeta) - \lambda c(\zeta, \xi)} \right]$$

Step 2

Take Away

$$\inf_{\theta\in\Theta} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[\ell(\theta,\xi)\right]$$

$$\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\Xi) : W_c(\mathbb{Q},\mathbb{P}) \leq \varepsilon\}$$

Step 1

$$\sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[\ell(\theta,\xi)\right] = \inf_{\lambda\geq 0} \lambda\varepsilon + \mathbb{E}_{\mathbb{P}}\left[\boxed{\sup_{\zeta\in\Xi} \ell(\theta,\zeta) - \lambda c(\zeta,\xi)}\right]$$

Step 2

References

[**BK16]** J. Blanchet,Y. Kang. Sample out-of-sample inference based on Wasserstein distance. OR, 2021.

[BKM19] J. Blanchet, Y. Kang, K. Murthy. Robust Wasserstein profile inference and applications to machine learning. JAP, 2019.

[BM19] J. Blanchet, K. Murthy. Quantifying distributional model risk via optimal transport. MOR, 2019.

[BMN21] J. Blanchet, K. Murthy, V. A. Nguyen. Statistical Analysis of Wasserstein Distributionally Robust Estimators. Tutorials in OR, 2021.

[BMZ18] J. Blanchet, K. Murthy, F. Zhang. Optimal transport based distributionally robust optimization: Structural properties and iterative schemes. MOR, 2021.

[CP18] R. Chen, I. C. Paschalidis. A robust learning approach for regression models based on distributionally robust optimization. JMLR, 2018.

[G90] M. Gelbrich, On a formula for the L2 Wasserstein metric between measures on Euclidean and Hilbert spaces, MN, 1990.

[G20] R. Gao. Finite-Sample Guarantees for Wasserstein Distributionally Robust Optimization: Breaking the Curse of Dimensionality. arXiv, 2020.

[GCK17] R. Gao, X. Chen, A. J. Kleywegt. Wasserstein distributionally robust optimization and variation regularization. arXiv, 2017.

[GK16] R. Gao, A. J. Kleywegt. Distributionally robust stochastic optimization with Wasserstein distance. arXiv, 2016.

[GSS15] I. J. Goodfellow, J. Shlens, C. Szegedy. Explaining and harnessing adversarial examples. In ICLR, 2015

[H-NW20] N. Ho-Nguyen, S. J. Wright. Adversarial Classification via Distributional Robustness with Wasserstein Ambiguity. MP, 2022.

[MK18] P. Mohajerin Esfahani, D. Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric. MP, 171(1- 2):115–166, 2018.

[NSKM21] V. A. Nguyen, S. Shafieezadeh-Abadeh, D. Kuhn, P. Mohajerin Esfahani. Bridging Bayesian and minimax mean square error estimation via Wasserstein distributionally robust optimization. MOR, 2021.

[S01] A. Shapiro. On duality theory of conic linear problems. In Semi-infinite Programming. Springer, 2001.

[SADK22] S. Shafieezadeh-Abadeh, L. Aolaritei, F. Dörfler, D. Kuhn. Optimal Transport Based Distributionally Robust Optimization: Nash Equilibrium and Regularization, Working Paper, 2022.

[SKM19] S. Shafieezadeh-Abadeh, D. Kuhn, and P. Mohajerin Esfahani. Regularization via Mass Transportation. JMLR, 2019.

[SMK15] S. Shafieezadeh-Abadeh, P. Mohajerin Esfahani, and D. Kuhn. Distributionally robust logistic regression. In NeurIPS 2015.

[TPJR18] Y. Tian, K. Pei, S. Jana, and B. Ray. Deeptest: Automated testing of deep-neural-network-driven autonomous cars. In ICSE, 2018.

[TSK2022] B. Taskesen, S. Shafieezadeh-Abadeh, D. Kuhn. Semi-discrete optimal transport: Hardness, regularization and numerical solution, MP, 2022.

[ZG18] C. Zhao and Y. Guan. Data-driven risk-averse stochastic optimization with Wasserstein metric. ORL, 2018.

[ZYG22] L. Zhang, J. Yang, and R. Gao. A Simple Duality Proof for Wasserstein Distributionally Robust Optimization. arXiv, 2022.

Optimality of Affine Hypotheses

Minimum Mean Square Error Estimator

$$J^\star = \inf_{h \in \mathbb{H}} \ \mathbb{E}_{\mathbb{P}}\left[\|h(x) - y\|_2^2\right]$$

$$\mathbb{H} = \{h : \mathbb{R}^n \to \mathbb{R}^m\}$$

Minimum Mean Square Error Estimator

$$J^\star = \inf_{h \in \mathbb{H}} \ \mathbb{E}_{\mathbb{P}}\left[\|h(x) - y\|_2^2\right]$$

Optimizer: $h^\star(x) = \mathbb{E}_{\mathbb{P}}[y \mid x]$

Optimal value: $J^\star = \operatorname{Tr}\left(\mathbb{COV}_{\mathbb{P}}[y \mid x]\right)$

MMSE under Normality

$$J^\star = \inf_{h \in \mathbb{H}} \mathbb{E}_{\mathbb{P}} \left[\|h(x) - y\|_2^2 \right] \qquad \& \qquad \mathbb{P} = \mathcal{N}(\mu, \Sigma)$$

Optimizer: $h^\star(x) = \mathbb{E}_{\mathbb{P}}[y \mid x]$

$$h^\star(x) = \Sigma_{yx} \Sigma_{xx}^{-1} (x - \mu_x) + \mu_y$$

Optimal value: $J^\star = \mathrm{Tr}\left(\mathbb{COV}_{\mathbb{P}}[y \mid x]\right)$

$$J^\star = \mathrm{Tr}\left[\Sigma_{yy} - \Sigma_{yx} \Sigma_{xx}^{-1} \Sigma_{xy}\right]$$

MMSE under Normality

$$J^\star = \inf_{h\in\mathbb{H}} \mathbb{E}_{\mathbb{P}}\left[\|h(x)-y\|_2^2\right]$$

MMSE under Normality

$$J^\star = \inf_{h \in \mathbb{H}} \; \mathbb{E}_{\mathbb{P}} \left[\| h(x) - y \|_2^2 \right]$$

Distributionally Robust MMSE Estimator

$$\inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \; \mathbb{E}_{\mathbb{Q}} \left[\|h(x) - y\|_2^2 \right]$$

$$\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\mathbb{X} \times \mathbb{Y}) : W_c(\mathbb{Q}, \mathbb{P}) \leq \varepsilon\}$$

$$\mathbb{P} = \mathcal{N}(\mu, \Sigma)$$

Distributionally Robust MMSE Estimator

$$\inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\|h(x) - y\|_2^2 \right]$$

$$\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\mathbb{X} \times \mathbb{Y}) : W_c(\mathbb{Q}, \mathbb{P}) \leq \varepsilon\}$$

$$\mathbb{P} = \mathcal{N}(\mu, \Sigma)$$

$$c\big((x, y), (x', y')\big) = \|(x, y) - (x', y')\|_2^2$$

Gelbrich Bound

Lemma 5. For any $\mathbb{Q}_1 \sim (\mu_1, \Sigma_1)$ and $\mathbb{Q}_2 \sim (\mu_2, \Sigma_2)$, we have

$$W_c\left(\mathbb{Q}_1, \mathbb{Q}_2\right) \geq \left\|\mu_1 - \mu_2\right\|^2 + \operatorname{Tr}\left[\Sigma_1 + \Sigma_2 - 2\left(\Sigma_2^{\frac{1}{2}} \Sigma_1 \Sigma_2^{\frac{1}{2}}\right)^{\frac{1}{2}}\right]$$

[G90]

Gelbrich Bound

Lemma 5. For any $\mathbb{Q}_1 \sim (\mu_1, \Sigma_1)$ and $\mathbb{Q}_2 \sim (\mu_2, \Sigma_2)$, we have

$$W_c(\mathbb{Q}_1, \mathbb{Q}_2) \geq \|\mu_1 - \mu_2\|^2 + \mathrm{Tr}\left[\Sigma_1 + \Sigma_2 - 2\left(\Sigma_2^{\frac{1}{2}} \Sigma_1 \Sigma_2^{\frac{1}{2}}\right)^{\frac{1}{2}}\right]$$

Tight under Normality.

[G90]

Gelbrich Bound

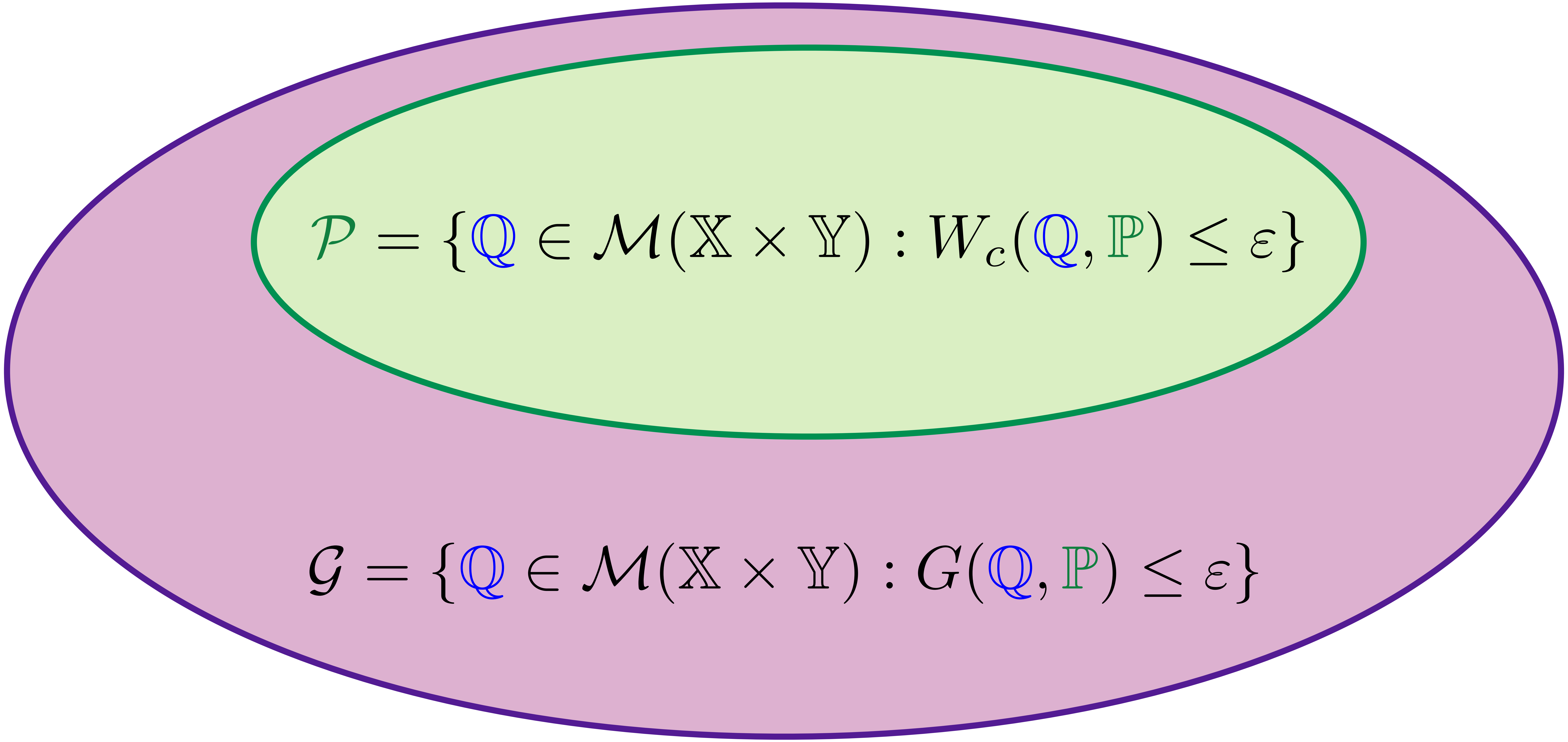
Lemma 5. For any $\mathbb{Q}_1 \sim (\mu_1, \Sigma_1)$ and $\mathbb{Q}_2 \sim (\mu_2, \Sigma_2)$, we have

$$W_c(\mathbb{Q}_1, \mathbb{Q}_2) \geq \boxed{\|\mu_1 - \mu_2\|^2 + \operatorname{Tr}\left[\Sigma_1 + \Sigma_2 - 2\left(\Sigma_2^{\frac{1}{2}} \Sigma_1 \Sigma_2^{\frac{1}{2}}\right)^{\frac{1}{2}}\right]}$$

Tight under Normality. $G(\mathbb{Q}_1, \mathbb{Q}_2)$

[G90]

Gelbrich Ambiguity Set



$$\mathcal{P} = \{\mathbb{Q} \in \mathcal{M}(\mathbb{X} \times \mathbb{Y}) : W_c(\mathbb{Q}, \mathbb{P}) \leq \varepsilon\}$$

$$\mathcal{G} = \{\mathbb{Q} \in \mathcal{M}(\mathbb{X} \times \mathbb{Y}) : G(\mathbb{Q}, \mathbb{P}) \leq \varepsilon\}$$

Useful Inequalities

$$\inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \ \mathbb{E}_{\mathbb{Q}} \left[\|h(x) - y\|_2^2 \right]$$

Useful Inequalities

$$\begin{aligned} & \inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \ \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] \\ \textbf{(restriction)} \qquad \leq \ & \inf_{h \in \mathbb{A}} \sup_{\mathbb{Q} \in \mathcal{P}} \ \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] \end{aligned}$$

Useful Inequalities

$$
\begin{aligned}
& && \inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\|h(x) - y\|_2^2 \right] \\
& \textbf{(restriction)} && \leq \inf_{h \in \mathbb{A}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\|h(x) - y\|_2^2 \right] \\
& \textbf{(Lemma 5)} && \leq \inf_{h \in \mathbb{A}} \sup_{\mathbb{Q} \in \mathcal{G}} \mathbb{E}_{\mathbb{Q}} \left[\|h(x) - y\|_2^2 \right]
\end{aligned}
$$

Useful Inequalities

$$\begin{aligned}
& \sup_{\mathbb{Q}\in\mathcal{P}} \inf_{h\in\mathbb{H}} \mathbb{E}_{\mathbb{Q}}\left[\|h(x)-y\|_2^2\right] \\
\textbf{(weak duality)} \quad & \leq \inf_{h\in\mathbb{H}} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[\|h(x)-y\|_2^2\right] \\
\textbf{(restriction)} \quad & \leq \inf_{h\in\mathbb{A}} \sup_{\mathbb{Q}\in\mathcal{P}} \mathbb{E}_{\mathbb{Q}}\left[\|h(x)-y\|_2^2\right] \\
\textbf{(Lemma 5)} \quad & \leq \inf_{h\in\mathbb{A}} \sup_{\mathbb{Q}\in\mathcal{G}} \mathbb{E}_{\mathbb{Q}}\left[\|h(x)-y\|_2^2\right]
\end{aligned}$$

Useful Inequalities

$$
\begin{aligned}
\sup_{\mathbb{Q} \in \mathcal{P} \cap \mathcal{N}} \inf_{h \in \mathbb{H}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] &\overset{\textbf{(restriction)}}{\leq} \sup_{\mathbb{Q} \in \mathcal{P}} \inf_{h \in \mathbb{H}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] \\
\textbf{(weak duality)} \quad &\leq \inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] \\
\textbf{(restriction)} \quad &\leq \inf_{h \in \mathbb{A}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] \\
\textbf{(Lemma 5)} \quad &\leq \inf_{h \in \mathbb{A}} \sup_{\mathbb{Q} \in \mathcal{G}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right]
\end{aligned}
$$

Sandwich Theorem

Theorem 5. We have

$$\sup_{\mathbb{Q} \in \mathcal{P} \cap \mathcal{N}} \inf_{h \in \mathbb{H}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right] = \inf_{h \in \mathbb{A}} \sup_{\mathbb{Q} \in \mathcal{G}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right]$$

[NSKM21]

Optimality of Affine Estimators

$$\boxed{\inf_{h \in \mathbb{H}} \sup_{\mathbb{Q} \in \mathcal{P}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right]} = \boxed{\sup_{\mathbb{Q} \in \mathcal{P}} \inf_{h \in \mathbb{H}} \mathbb{E}_{\mathbb{Q}} \left[\| h(x) - y \|_2^2 \right]}$$

$h^\star$ is affine

$\mathbb{Q}^\star$ is Normal

$$h^\star = \operatorname*{argmin}_{h \in \mathbb{H}} \mathbb{E}_{\mathbb{Q}^\star} \left[\| h(x) - y \|_2^2 \right]$$