Omnipredicting Single-Index Models with Multi-Index Models

Kevin Tian (UT Austin)

Simons Institute IFML/MPG Symposium

Based on joint work with:

Lunjia Hu (Harvard \rightarrow Northeastern), Chutong Yang (UT Austin)

Roadmap

- Overview
	- Omniprediction
	- SIMs
	- Our results
- Isotron
	- Realizable setting
	- Agnostic setting
- Efficient omniprediction
	- Sample complexity
	- Runtime complexity

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell(p(\mathbf{x}),y)\right] \le \min_{c\in\mathcal{C}}\left[\ell(c(\mathbf{x},y))\right] + \epsilon
$$

…traditional paradigm in supervised learning…

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The main characters:

• Distribution D over $\{x \in \mathbb{R}^d | ||x|| \leq 1\} \times \{0,1\}$

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- Comparator class C (e.g., linear functions)

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- Loss function ℓ (e.g., squared loss, cross entropy, …)

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- Distribution D over $\{x \in \mathbb{R}^d | ||x|| \leq 1\} \times \{0,1\}$
- Comparator class C (e.g., linear functions)
- Loss function ℓ (e.g., squared loss, cross entropy, …)
- Predictor p : can be *proper* $(p \in C)$ or *improper*

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What if loss not known in advance?

• Depends on parameters unknown at training

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$$

What if loss not known in advance?

- Depends on parameters unknown at training
- Multiple tasks (e.g., weights of false pos/neg)
- "Fundamental truth" of D independent of loss
	- Drives us closer to ground truth $p^*(\mathbf{x}) \coloneqq \mathbb{E}[y|\mathbf{x}]$

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell(k_{\ell}(p(\mathbf{x})),y)\right] \leq \min_{c \in \mathcal{C}}\left[\ell(c(\mathbf{x},y))\right] + \epsilon \qquad \forall \ell \in \mathcal{L}
$$

[Gopalan-Kalai-Reingold-Sharan-Wieder '22]

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell(k_{\ell}(p(\mathbf{x})),y)\right] \leq \min_{c \in \mathcal{C}}\left[\ell(c(\mathbf{x},y))\right] + \epsilon \qquad \forall \ell \in \mathcal{L}
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The additional characters:

• Loss function *family L* (e.g., proper losses)

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The additional characters:

- Loss function *family L* (e.g., proper losses)
- Loss-specific post-processings $\{k_{\ell}\}_{\ell \in \mathcal{L}}$
	- Distribution-independent
	- Role of p: "supervised sufficient statistics" for D

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- Loss function *family L* (e.g., proper losses)
- Loss-specific post-processings $\{k_{\ell}\}_{{\ell} \in {\ell}}$
	- Distribution-independent
	- Role of p: "supervised sufficient statistics" for D
- Fundamentally an *agnostic learning* guarantee!

$$
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$$

Idea I: multicalibration suffices [GKRSW '22]

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Idea 1: multicalibration suffices [GKRSW '22]

• Powerful property: agrees with ground truth on parameterized *conditional dists*

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- Reduce from *agnostically learning* C via iterative boosting [Hébert-Johnson-Kim-Reingold-Rothblum '18]

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- Powerful property: agrees with ground truth on parameterized *conditional dists*
- Reduce from *agnostically learning* C via iterative boosting [Hébert-Johnson-Kim-Reingold-Rothblum '18]
- Computationally-intractable in many settings… (e.g. halfspaces [Guruswami-Raghavendra '06, …])

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell(k_{\ell}(p(\mathbf{x})),y)\right] \leq \min_{c \in \mathcal{C}}\left[\ell(c(\mathbf{x},y))\right] + \epsilon \qquad \forall \ell \in \mathcal{L}
$$

Idea 2: weaker conditions suffice [Gopalan-Hu-Kim-Reingold-Wieder '23]

• "Statistical tests" parameterized by $C\times L$

$$
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$$

Idea 2: weaker conditions suffice [Gopalan-Hu-Kim-Reingold-Wieder '23]

- "Statistical tests" parameterized by $C\times L$
- Calibration + "multi-accuracy" suffice: improved quantitative bounds for explicit families

 $\mathbb{E}[y \mid \mathbf{x}] \approx \sigma(\mathbf{w} \cdot \mathbf{x})$ ___________

$$
\mathbb{E}[y \mid \mathbf{x}] \approx \sigma(\mathbf{w} \cdot \mathbf{x})
$$

\n"Semi-parametric" model family
\n• Parametric: linear predictor $\mathbf{w} \in \mathbb{W} \in \mathbb{R}^d ||\|\mathbf{w}\| \le 1$

$$
\begin{array}{c}\n\vdots \\
\downarrow\n\end{array}\n\begin{bmatrix}\n\mathbf{E}\left[y \mid \mathbf{x}\right] \approx \sigma(\mathbf{w} \cdot \mathbf{x}) \\
\vdots \\
\downarrow\n\end{bmatrix}
$$
\n"Semi-parametric" model family

- Parametric: *linear predictor* $\mathbf{w} \in \mathcal{W} \coloneqq {\mathbf{w} \in \mathbb{R}^d \,|\, ||\mathbf{w}|| \leq 1}$
- Non-parametric: *link function* $\sigma \in \mathcal{S} := \beta$ -Lipschitz, monotone functions σ : $[-1,1] \rightarrow [0,1]$
	- Known link: generalized linear model

Every link σ has...

…induced *matching loss*

 $\int_{0}^{1} \ell_{\mathsf{m},\sigma}(t,y) := \int_{0}^{t} (\sigma(\tau)-y) d\tau.$

Every link σ has...

…induced *matching loss*

$$
\iota_{\mathsf{m},\sigma}(t,y) := \int_0^t (\sigma(\tau) - y) \mathrm{d}\tau
$$
\n
$$
\frac{\partial}{\partial t} \ell_{\mathsf{m},\sigma}(t,y) = \sigma(t) - y
$$
\n
$$
\text{(convex)}
$$

Every link σ has...

…induced *matching loss*

$$
\begin{aligned}\n\text{...induced matching loss} & \qquad \downarrow \ell_{\mathsf{m},\sigma}(t,y) := \int_0^t (\sigma(\tau) - y) \, \mathrm{d}\tau \, \Big| \\
\text{...} & \qquad \qquad \downarrow \\
\sigma^{-1}(\mathbb{E}[y]) \in \operatorname{argmin}_t \{ \ell_{\mathsf{m},\sigma}(t,y) \} & \iff \frac{\partial}{\partial t} \ell_{\mathsf{m},\sigma}(t,y) = \sigma(t) - y\n\end{aligned}
$$

(convex)

Every link σ has...

…induced *matching loss*

…induced *proper loss*

$$
\ell_{\mathsf{m},\sigma}(t,y) := \int_0^t (\sigma(\tau) - y) \mathrm{d}\tau \cdot \frac{1}{\tau}
$$
\n
$$
\frac{1}{\tau} \cdot \ell_{\mathsf{p},\sigma}(v,y) := \ell_{\mathsf{m},\sigma}(\sigma^{-1}(v),y) \cdot \frac{1}{\tau}
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\n
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\n
$$
\frac{1}{\tau} \cdot \ell_{\mathsf{p},\sigma}(v,y) := \ell_{\mathsf{m},\sigma}(\sigma^{-1}(v),y) \cdot \frac{1}{\tau}
$$
\n(if y ~ Bernoulli, minimized by ground truth)

$$
\sigma(\mathbf{w}\cdot\mathbf{x})=\mathbb{E}[y\mid\mathbf{x}]
$$

Isotron learns SIMs!

[Kalai-Sastry '09, Kakade-Kalai-Kanade-Shamir '11]

realizable

$$
\sigma(\mathbf{w}\cdot\mathbf{x})=\mathbb{E}[y\mid\mathbf{x}]
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- Very simple algo (gradient descent + isotonic regression)
- Proper hypotheses

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\sigma(\mathbf{w}\cdot\mathbf{x})\approx^? \mathbb{E}[y\mid\mathbf{x}]
$$

"Constant-factor" learners

[Gollakota-Gopalan-Klivans-Stavropoulos '23, Zarifis-Wang-Diakonikolasx2 '24]

agnostic

$$
\sigma(\mathbf{w}\cdot\mathbf{x})=\mathbb{E}[y\mid\mathbf{x}]
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Isotron learns SIMs!

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- Very simple algo (gradient descent + isotonic regression)
- Proper hypotheses

 $\sigma(\mathbf{w} \cdot \mathbf{x}) \approx^? \mathbb{E}[y | \mathbf{x}]$

"Constant-factor" learners

- [Gollakota-Gopalan-Klivans-Stavropoulos '23, Zarifis-Wang-Diakonikolasx2 '24]
- More distributional assumptions, structure (e.g. bi-Lipschitz, anti-conc.)
- Very large overheads (e.g., [ZWDD24] needs $d\kappa^{44}$ samples)

agnostic

Our goal: for all $(\sigma, w) \in S\times W...$ $\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}\left(k_{\sigma}(p(\mathbf{x})),y\right)\right]\leq\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}\left(\mathbf{w}\cdot\mathbf{x},y\right)\right]+\epsilon$

Our goal: for all $(\sigma, w) \in S\times W...$ $\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}\left(k_{\sigma}(p(\mathbf{x})),y\right)\right]\leq\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}\left(\mathbf{w}\cdot\mathbf{x},y\right)\right]+\epsilon$

…another view when *p* scalar…

$$
\mathbb{E}_{(\mathbf{x},y)}\left[\ell_{\mathbf{p},\sigma}(p(\mathbf{x}),y)\right]\leq \mathbb{E}_{(\mathbf{x},y)}\left[\ell_{\mathbf{p},\sigma}(\sigma(\mathbf{w}\cdot\mathbf{x}),y)\right]
$$

"competing with all (proper) SIMs"

Our goal: for all $(\sigma, w) \in S\times W$... $\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}\left(k_{\sigma}(p(\mathbf{x})),y\right)\right]\leq \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}\left(\mathbf{w}\cdot\mathbf{x},y\right)\right]+\epsilon$

Existing construction [GHKRW '23]: $\approx \epsilon^{-10}$ samples

Iterate until MA and CAL:

- Calibrated residual
	- Bucket + estimate quantiles
- Multiaccurate residual
	- Repeated truncation + boosting

$$
\text{Our goal: for all } (\sigma, \mathbf{w}) \in S \times \mathcal{W} \dots
$$
\n
$$
\mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[\ell_{\mathsf{m}, \sigma} \left(k_{\sigma}(p(\mathbf{x})), y \right) \right] \leq \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[\ell_{\mathsf{m}, \sigma} \left(\mathbf{w} \cdot \mathbf{x}, y \right) \right] + \epsilon
$$

Existing construction [GHKRW '23]: $\approx \epsilon^{-10}$ samples

- Complex algo / hypothesis
	- Highly-improper (interpretability?)
	- Large sequential depth

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$$

Existing construction [GHKRW '23]: $\approx \epsilon^{-10}$ samples

- Complex algo / hypothesis
	- Highly-improper (interpretability?)
	- Large sequential depth
- Loose sample / runtime complexity?

Iterate until MA and CAL:

- Calibrated residual
	- Bucket + estimate quantiles
- Multiaccurate residual
	- Repeated truncation + boosting
Philosophy

"TCS"-style results

- Challenging setup (agnostic, heterogeneous, nonconvex, …)
- Provable guarantees!!!
- Polynomial time / samples!!!

Philosophy

…okay, but what polynomial?

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Philosophy

…okay, but what polynomial?

"TCS"-style results

- Challenging setup (agnostic, heterogeneous, nonconvex, …)
- Provable guarantees!!!
- Polynomial time / samples!!!

Strive for "right" algorithms, analyses in tractable settings to make impact on applications.

Theorem [HTY '24]: There is an omnipredictor for SIMs using…

- β^2 $\frac{\rho}{\epsilon^4}$ samples (for β -Lipschitz, monotone links)
	- $\cdot \frac{\beta^2}{\beta^2}$ $\frac{P}{\alpha^2 \epsilon^2}$ samples (for (α, β) -bi-Lipschitz links)

...in nearly-linear time
$$
\tilde{O}(nd \cdot \epsilon^{-2})
$$

Theorem [HTY '24]: There is an omnipredictor for SIMs using…

• β^2 $\frac{\rho}{\epsilon^4}$ samples (for β -Lipschitz, monotone links) $\cdot \frac{\beta^2}{\beta^2}$ $\frac{P}{\alpha^2 \epsilon^2}$ samples (for (α, β) -bi-Lipschitz links)

…with the "multiindex model" form

$$
p(\mathbf{x}) = {\{\sigma_t(\mathbf{w}_t \cdot \mathbf{x})\}_{t \in [O(\epsilon^{-2})]}}
$$

Theorem [HTY '24]: There is an omnipredictor for SIMs using…

• β^2 $\frac{\rho}{\epsilon^4}$ samples (for β -Lipschitz, monotone links) $\cdot \frac{\beta^2}{\beta^2}$ $\frac{P}{\alpha^2 \epsilon^2}$ samples (for (α, β) -bi-Lipschitz links)

The algo is Isotron with custom iso-reg solver + post-processing. We call it the *Omnitron*.

"ERM" omniprediction

Better time / sample complexities (second moment bound)

Same results existentially hold for population-level omniprediction

Omnipredicting SIMs in R

Theorem [HTY '24]: Two SIMs suffice ("double-index model")

Open Q: is there a proper omnipredictor, even in 1-d?

Roadmap

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- SIMs
- Our results

• Isotron

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- Agnostic setting
- Efficient omniprediction
	- Sample complexity
	- Runtime complexity

Isotron

Isotron

Algorithm 1: $\mathsf{Isotron}(\mathcal{D},T,\eta)$

- 1 **Input:** Distribution D from Model 2, iteration count $T \in \mathbb{N}$, step size $\eta > 0$
- 2 $\mathbf{w}_0 \leftarrow \mathbf{0}_d$ 3 for $0 \le t < T$ do $\sigma_t \leftarrow \argmin_{\sigma \in \mathcal{S}_{0,\beta}} \{\ell_{\textsf{sq}}(\sigma, \mathbf{w}_t; \mathcal{D})\}$ $\overline{\mathbf{4}}$ $\mathbf{w}_{t+1} \leftarrow \mathbf{\Pi}_{\mathcal{W}}(\mathbf{w}_t - \eta \nabla_{\mathbf{w}} \ell_{\mathsf{m}, \sigma_t}(\mathbf{w}_t; \mathcal{D}))$ $\bf{5}$ 6 end 7 return $\{\sigma_t\}_{0 \leq t \leq T-1}, \{\mathbf{w}_t\}_{0 \leq t \leq T}$

Isotron

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1 **Input:** Distribution D from Model 2, iteration count $T \in \mathbb{N}$, step size $\eta > 0$

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$$
\mathbf{w}_0 \leftarrow \mathbf{0}_d
$$

\n3 for $0 \le t < T$ do
\n4 $\sigma_t \leftarrow \arg \min_{\sigma \in \mathcal{S}_{0,\beta}} \{\ell_{sq}(\sigma, \mathbf{w}_t; \mathcal{D})\}$
\n5 $\mathbf{w}_{t+1} \leftarrow \Pi_{\mathcal{W}}(\mathbf{w}_t - \eta \nabla_{\mathbf{w}} \ell_{m, \sigma_t}(\mathbf{w}_t; \mathcal{D}))$
\n6 end
\n7 return $\{\sigma_t\}_{0 \le t \le T-1}, \{\mathbf{w}_t\}_{0 \le t \le T}$

$$
\ell_{\mathsf{sq}}(\sigma, \mathbf{w}; \mathcal{D}) := \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(\sigma(\mathbf{w} \cdot \mathbf{x}) - y)^2 \right]
$$

$$
\nabla_{\mathbf{w}} \ell_{\mathbf{m}, \sigma}(\mathbf{w}; \mathcal{D}) = \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(\sigma(\mathbf{w} \cdot \mathbf{x}) - y) \cdot \mathbf{x} \right]
$$

 $\lfloor \nu_i \rfloor \cup \leq i \leq 1-1$, $\lfloor \nu_i \rfloor \cup \leq i \leq 1$

Idea 1: regret minimization

$$
\frac{1}{T} \sum_{0 \leq t < T} \langle \nabla_{\mathbf{w}} \ell_{\mathbf{m}, \sigma_t} (\mathbf{w}_t; \mathcal{D}), \mathbf{w}_t - \mathbf{w} \rangle \leq \epsilon
$$

Idea 2: optimality of iso-reg

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t;\mathcal{D}),\mathbf{w}_t-\mathbf{w}\rangle = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t\cdot\mathbf{x})-y)(\mathbf{w}_t\cdot\mathbf{x}-\mathbf{w}\cdot\mathbf{x})\right]
$$

Idea 2: optimality of iso-reg

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t; \mathcal{D}), \mathbf{w}_t - \mathbf{w} \rangle = \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \mathbf{w} \cdot \mathbf{x}) \right]
$$

\n
$$
= \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x})) \right]
$$

\n
$$
+ \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

Idea 2: optimality of iso-reg

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t; \mathcal{D}), \mathbf{w}_t - \mathbf{w} \rangle = \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \mathbf{w} \cdot \mathbf{x}) \right]
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$$

\n
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+ \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x}) \right] \right]
$$

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x})\right]
$$
\n
$$
\geq \mathbb{E}_{\mathbf{x}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - \sigma(\mathbf{w} \cdot \mathbf{x}))^2\right]
$$
\n(excess squared loss)

Idea 2: optimality of iso-reg

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t;\mathcal{D}),\mathbf{w}_t-\mathbf{w} \rangle = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \mathbf{w} \cdot \mathbf{x}) \right] \n= \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x})) \right] \n+ \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x})) \right] = 0
$$

(iso-reg solution calibrated)

Idea 2: optimality of iso-reg

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t; \mathcal{D}), \mathbf{w}_t - \mathbf{w} \rangle = \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \mathbf{w} \cdot \mathbf{x}) \right]
$$

\n
$$
= \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x})) \right]
$$

\n
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+ \mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

\n
$$
\geq \ell_{\mathsf{sq}}(\sigma_t, \mathbf{w}_t; \mathcal{D}) - \ell_{\mathsf{sq}}(\sigma, \mathbf{w}; \mathcal{D})
$$

…some iterate is good, i.e., proper learner

Isotron analysis (agnostic setting)

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t;\mathcal{D}),\mathbf{w}_t-\mathbf{w}\rangle = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t\cdot\mathbf{x})-y)(\mathbf{w}_t\cdot\mathbf{x}-\mathbf{w}\cdot\mathbf{x})\right] \n= \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t\cdot\mathbf{x})-y)(\mathbf{w}_t\cdot\mathbf{x}-\sigma^{-1}(\mathbf{w}_t\cdot\mathbf{x}))\right] \n+ \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t\cdot\mathbf{x})-y)(\sigma^{-1}(\mathbf{w}_t\cdot\mathbf{x})-\mathbf{w}\cdot\mathbf{x})\right]
$$

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x}) \right] \ge 0
$$

…still OK by KKT conditions of *Lipschitz* iso-reg! [Lemma 1, KKKS '11]

Isotron analysis (agnostic setting)

$$
\langle \nabla_{\mathbf{w}} \ell_{\mathbf{m},\sigma_t}(\mathbf{w}_t;\mathcal{D}),\mathbf{w}_t-\mathbf{w}\rangle = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x}-\mathbf{w} \cdot \mathbf{x})\right]
$$

$$
= \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x}-\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}))\right]
$$

$$
+ \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x}) - \mathbf{w} \cdot \mathbf{x})\right] \right]
$$

What about…

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(\sigma_t(\mathbf{w}_t \cdot \mathbf{x}) - y)(\mathbf{w}_t \cdot \mathbf{x} - \sigma^{-1}(\mathbf{w}_t \cdot \mathbf{x})) \right]
$$

$$
\mathsf{OG}(p) := \sup_{(\mathbf{w}, \sigma) \in \mathcal{W} \times \mathcal{S}} \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(p(\mathbf{x}) - y)(\sigma^{-1}(p(\mathbf{x})) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

$$
\mathsf{OG}(p) := \sup_{(\mathbf{w}, \sigma) \in \mathcal{W} \times \mathcal{S}} \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(p(\mathbf{x}) - y)(\sigma^{-1}(p(\mathbf{x})) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

Ground truth *p* has zero omnigap!

Interpretation: small omnigap \rightarrow passing many "indistinguishability" statistical tests

"calibration"

$$
\mathsf{OG}(p) := \sup_{(\mathbf{w}, \sigma) \in \mathcal{W} \times \mathcal{S}} \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(p(\mathbf{x}) - y)(\sigma^{-1}(p(\mathbf{x})) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

"multi-accuracy"

…turns out to be a one-sided variant of "loss outcome indistinguishability" [GHKRW '23]

$$
\mathsf{OG}(p) := \sup_{(\mathbf{w}, \sigma) \in \mathcal{W} \times \mathcal{S}} \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(p(\mathbf{x}) - y)(\sigma^{-1}(p(\mathbf{x})) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

Theorem [implicit, GHKRW '23]:

 $\mathsf{OG}(p) \leq \epsilon \implies p$ is an ϵ -omnipredictor for SIMs

Proof. Let $\hat{\mathcal{D}}$ be the distribution on $\mathcal{X} \times \{0,1\}$ which draws $\mathbf{x} \sim \mathcal{D}_{\mathbf{x}}$ and then $y \mid \mathbf{x} \sim \text{Bern}(p(\mathbf{x}))$. We have that the following hold, because the integral part of Definition 1 cancels in each line:

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathbf{p},\sigma}(p(\mathbf{x}),y)\right] - \mathbb{E}_{(\mathbf{x},y)\sim\hat{\mathcal{D}}}\left[\ell_{\mathbf{p},\sigma}(p(\mathbf{x}),y)\right] = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\left(p(\mathbf{x})-y\right)\sigma^{-1}\left(p(\mathbf{x})\right)\right],
$$

$$
\mathbb{E}_{(\mathbf{x},y)\sim\hat{\mathcal{D}}}\left[\ell_{\mathbf{m},\sigma}(\mathbf{w}\cdot\mathbf{x},y)\right] - \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathbf{m},\sigma}(\mathbf{w}\cdot\mathbf{x},y)\right] = - \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\left(p(\mathbf{x})-y\right)(\mathbf{w}\cdot\mathbf{x})\right].
$$

Moreover, by the definition of $\widehat{\mathcal{D}}$ (i.e., labels are $\sim \text{Bern}(p(\mathbf{x}))$), because $\ell_{p,\sigma}$ is a proper loss,

$$
E_{(\mathbf{x},y)\sim \widehat{\mathcal{D}}} \left[\ell_{\mathbf{p},\sigma}(p(\mathbf{x}),y)\right]-\mathbb{E}_{(\mathbf{x},y)\sim \widehat{\mathcal{D}}} \left[\ell_{\mathbf{m},\sigma}(\mathbf{w}\cdot \mathbf{x},y)\right]\leq 0.
$$

Summing up the above displays, we obtain for any $(\sigma, \mathbf{w}) \in S \times W$,

$$
\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{p},\sigma}(p(\mathbf{x}),y)\right] - \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell_{\mathsf{m},\sigma}(\mathbf{w}\cdot\mathbf{x},y)\right] \leq \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[(p(\mathbf{x})-y)(\sigma^{-1}(p(\mathbf{x}))-\mathbf{w}\cdot\mathbf{x})] \n= \mathsf{OG}(p;\sigma,\mathbf{w}).
$$
\n(13)

Because (σ, \mathbf{w}) were arbitrary, by using $\mathsf{OG}(p) \leq \varepsilon$, we have the claim. $\overline{}$

$$
\mathsf{OG}(p) := \sup_{(\mathbf{w}, \sigma) \in \mathcal{W} \times \mathcal{S}} \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(p(\mathbf{x}) - y)(\sigma^{-1}(p(\mathbf{x})) - \mathbf{w} \cdot \mathbf{x}) \right]
$$

Yields a new, simpler proof of PAV optimality in 1-d (key ingredient in our 1-d omnipredictor construction)

Omnitron

Algorithm 3: Omnitron($\{(\mathbf{x}_t, y_t)\}_{0 \leq t < T}, T, \eta, \mathcal{O}, \varepsilon$)

1 Input: $\{(\mathbf{x}_t, y_t)\}_{0 \leq t \leq T} \sim_{i.i.d.} \mathcal{D}$ for a distribution \mathcal{D} from Model 2, iteration count $T \in \mathbb{N}$, step size $\eta > 0$, ε -approximate BIR oracle \mathcal{O} (Definition 6) 2 $\mathbf{w}_0 \leftarrow \mathbf{0}_d$ 3 for $0 \leq t \leq T$ do $4 \mid \sigma_t \leftarrow \mathcal{O}(\mathbf{w}_t)$ (rest of talk)5 $\tilde{\mathbf{g}}_t \leftarrow (\sigma_t(\mathbf{w}_t \cdot \mathbf{x}_t) - y_t)\mathbf{x}_t$ ("adaptive" stochastic optimization) 6 $\mathbf{w}_{t+1} \leftarrow \mathbf{\Pi}_{\mathcal{W}}(\mathbf{w}_t - \eta \tilde{\mathbf{g}}_t)$ 7 end 8 return $p: \mathbf{x} \to \{\sigma_t(\mathbf{w}_t \cdot \mathbf{x})\}_{0 \leq t \leq T-1}, k_{\sigma} : \{p_t\}_{0 \leq t < T} \to \frac{1}{T} \sum_{0 \leq t < T} \sigma^{-1}(p_t)$

Roadmap

• Overview

- Omniprediction
- SIMs
- Our results
- Isotron
	- Realizable setting
	- Agnostic setting
- Efficient omniprediction
	- Sample complexity
	- Runtime complexity

Robust omniprediction

For input
$$
\widehat{\mathbf{w}} \in \mathcal{W}
$$
 return $\widehat{\sigma} \in \mathcal{S}$ s.t. for all $\sigma \in \mathcal{S}$
\n
$$
\mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} \left[(\widehat{\sigma}(\widehat{\mathbf{w}} \cdot \mathbf{x}) - y)(\mathbf{w} \cdot \mathbf{x} - \sigma^{-1}(\widehat{\sigma}(\mathbf{w} \cdot \mathbf{x}))) \right] \ge -\epsilon
$$

Robust omniprediction

For input
$$
\widehat{\mathbf{w}} \in \mathcal{W}
$$
 return $\widehat{\sigma} \in \mathcal{S}$ s.t. for all $\sigma \in \mathcal{S}$
\n
$$
\mathbb{E}_{(\mathbf{x},y) \sim \mathcal{D}} [(\widehat{\sigma}(\widehat{\mathbf{w}} \cdot \mathbf{x}) - y)(\mathbf{w} \cdot \mathbf{x} - \sigma^{-1}(\widehat{\sigma}(\mathbf{w} \cdot \mathbf{x})))] \ge -\epsilon
$$
\n(population-level iso-reg suffices but intractable)

Robust omniprediction

For input
$$
\widehat{\mathbf{w}} \in \mathcal{W}
$$
 return $\widehat{\sigma} \in \mathcal{S}$ s.t. for all $\sigma \in \mathcal{S}$

$$
\mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[(\widehat{\sigma}(\widehat{\mathbf{w}} \cdot \mathbf{x}) - y)(\mathbf{w} \cdot \mathbf{x} - \sigma^{-1}(\widehat{\sigma}(\mathbf{w} \cdot \mathbf{x}))) \right] \ge -\epsilon
$$

(population-level iso-reg suffices but intractable)

$$
\approx \mathbb{E}_{(\mathbf{x},y)\sim\widehat{\mathcal{D}}_n} \left[(\widehat{\sigma}(\widehat{\mathbf{w}} \cdot \mathbf{x}) - y)(\mathbf{w} \cdot \mathbf{x} - \sigma^{-1}(\widehat{\sigma}(\mathbf{w} \cdot \mathbf{x}))) \right]
$$

Key ideas for uniform convergence:

- Smoothing (slightly anti-Lipschitz w.l.o.g.)
	- Dudley's generic chaining

$$
\min_{\{v_i\}_{i \in [n]} \subseteq \mathbb{R}} \sum_{i \in [n]} (v_i - y_i)^2
$$
\n
$$
\text{s.t.} \qquad a_i \le v_{i+1} - v_i \le b_i \text{ for all } i \in [n-1]
$$

(empirical "bounded" iso-reg)

 $\min_{\{v_i\}_{i\in[n]}\subseteq\mathbb{R}}\sum_{i\in[n]}(v_i-y_i)^2$ $a_i \le v_{i+1} - v_i \le b_i$ for all $i \in [n-1]$ s.t. anti-Lipschitz / Lipschitz monotonicity constraints constraints

(also in [KKKS '11, ZWDD '24])

$$
\min_{\{v_i\}_{i \in [n]} \subseteq \mathbb{R}} \sum_{i \in [n]} (v_i - y_i)^2
$$
\n
$$
\text{s.t.} \qquad a_i \le v_{i+1} - v_i \le b_i \text{ for all } i \in [n-1]
$$

Prev. solver: inexact, $\Omega(n^2)$ time [HTY '24]: exact, $O(n(\log(n))^2)$ Fast DP on piecewise quadratic

$$
\min_{\{v_i\}_{i \in [n]} \subseteq \mathbb{R}} \sum_{i \in [n]} (v_i - y_i)^2
$$
\ns.t.

\n
$$
a_i \le v_{i+1} - v_i \le b_i \text{ for all } i \in [n-1]
$$

Prev. solver: inexact, $\Omega(n^2)$ time [HTY '24]: exact, $O(n(\log(n))^2)$ Fast DP on piecewise quadratic

Testing Calibration in Nearly-Linear Time [Hu-Jambulapati-Tian-Yang '24] See Chutong's poster!

What else?

- 1. Omnipredicting structured families?
	- Regression setting?
	- Multi-class classification?
	- Multi-objective optimization? (Thanks Han \circledcirc)
- 2. Proper omnipredictors?
	- Do they exist?
	- Some partial characterizations in our paper…
- 3. Practical implications?
	- Multigroup fairness, e.g., for fine-tuning

Thank you!

Contact kjtian.github.io kjtian@cs.utexas.edu

