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The Implicit Bias of Benign Overfitting

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Outline

Introduction

Regression

Beyond square loss

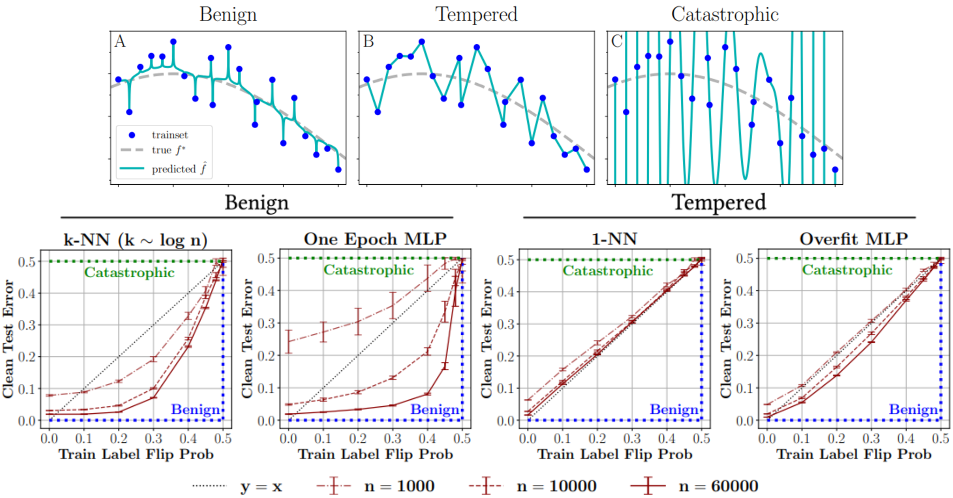
Classification

Zhang, Chiyuan et al. “Understanding deep learning requires rethinking generalization.” ArXiv abs/1611.03530 (2016): n. pag.

Zhang, Chiyuan, et al. ”Understanding deep learning (still) requires rethinking generalization.” Communications of the ACM 64.3 (2021): 107-115.

- Deep architectures are able to (and often do) memorize whole datasets...
- ...but traditional generalization bounds fail to explain their performance.
- Sparked research: tighter generalization bounds, interpolating regime, double descent, benign overfitting, implicit versus explicit regularization

Mallinar, Neil, et al. "Benign, tempered, or catastrophic: A taxonomy of overfitting." arXiv preprint arXiv:2207.06569 (2022).



Notation and setting

- $\{\mathcal{D}_d\}_{d=k+1}^{\infty}$ sequence of distributions on $\mathbb{R}^d \times Y$
  - $Y = \mathbb{R}$ for regression and $Y = \{-1, 1\}$ for classification
- If $(\mathbf{x}, y) \sim \mathcal{D}_d$, then
  - $\mathbf{x}_{|k} \in \mathbb{R}^k$ follows a (fixed) arbitrary distribution
  - $\mathbf{x}_{|d-k} \in \mathbb{R}^{d-k}$ follows a (changing) high-dimensional distribution; "junk features"
- sample sizes $\{m_d\}_{d=k+1}^{\infty}$ and IID samples $\{(\mathbf{x}_i, y_i)\}_{i=1}^{m_d}$ from $\mathcal{D}_d$ for each d
- Consider linear predictors $\mathbf{w} \in \mathbb{R}^d$ evaluated as $\mathbf{x} \mapsto \mathbf{x}^T\mathbf{w}$ or $\mathbf{x} \mapsto \mathrm{sign}(\mathbf{x}^T\mathbf{w})$

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Min-norm interpolating predictors

- empirical loss $L_d(\mathbf{w}) := \frac{1}{m_d} \sum_{i=1}^{m_d} \left(\mathbf{x}_i^T \mathbf{w} - y_i\right)^2$
- true risk $R_d(\mathbf{w}) := \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}_d} \left[\left(\mathbf{x}^T \mathbf{w} - y\right)^2\right]$
- Under mild conditions, iterative training methods with interpolating output converge to the min-norm predictor

$$\hat{\mathbf{w}} := \arg\min_{\mathbf{w}\in\mathbb{R}^d} \|\mathbf{w}\| : L_d(\mathbf{w}) = 0$$

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Benign overfitting

A sequence of distributions $\{\mathcal{D}_d\}_{d=k+1}^{\infty}$ satisfies benign overfitting if there is a sequence of sample sizes $\{m_d\}_{d=k+1}^{\infty}$ such that

- $\Pr\{L_d(\mathbf{w}) = 0\} \to 1$ as $d \to \infty$,
- $\inf_d \inf_{\mathbf{w}\in\mathbb{R}^d} R_d(\mathbf{w}) > 0$, and
- with the min-norm predictor $\hat{\mathbf{w}}_d$ we have

$$R_d(\hat{\mathbf{w}}_d) - \inf_{\mathbf{w}\in\mathbb{R}^d} R_d(\mathbf{w}) \xrightarrow{P} 0$$

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The well-specified case

Bartlett, Peter L., et al. "Benign overfitting in linear regression." Proceedings of the National Academy of Sciences 117.48 (2020): 30063-30070.

Assume $\mathbb{E}[y \mid \mathbf{x}] = \mathbf{x}^T \mathbf{w}^*$ and let $\mathbf{x}$ have zero mean. Let $\Sigma = \Sigma_k \oplus \Sigma_{d-k}$ be the covariance matrix split along eigenvectors. Then, benign overfitting necessarily implies that

$$m \cdot \frac{\|\Sigma_{d-k}\|_F^2}{\mathrm{Tr}^2(\Sigma_{d-k})} \to 0$$

Lemma

If $\mathbf{z}, \mathbf{z}'$ are IID random vectors such that $\mathbb{E}[\mathbf{z}\mathbf{z}^T] = \Sigma$, then $\mathbb{E}[\mathbf{z}^T \mathbf{z}'] = \|\Sigma\|_F^2$.
Consequently, if $m \cdot \|\Sigma\|_F^2 / \mathrm{Tr}^2(\Sigma) \to 0$, then also $m \cdot \frac{\mathbb{E}[(\mathbf{z}\mathbf{z}')^2]}{\mathbb{E}^2[\|\mathbf{z}\|^2]} \to 0$.

- Even in a well-specified setting we need high-dimensional distributions producing samples with almost orthogonal directions.

Deterministic perturbation bound

Let $\{(\mathbf{x}_i, y_i\}_{i=1}^m$ be a deterministic sample of size m. Define the perturbation matrix

$$E_{ij} := \mathbf{x}_{i|d-k}^T \mathbf{x}_{j|d-k} \cdot \mathbf{1}\{i \neq j\} \in \mathbb{R}^{m \times m}.$$

Assume that the $\{\mathbf{x}_i\}_{i=1}^m$ are linearly independent,

$$\frac{\|E\|}{\min_i \|\mathbf{x}_{i|d-k}\|^2} \leq \frac{1}{2}, \quad \text{and} \quad \frac{1}{2} \leq \frac{1}{2}\lambda_{\min}\left(\hat{\mathbb{E}}\left[\frac{\mathbf{x}_{|k}\mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2}\right]\right).$$

Then, the min-norm predictor $\hat{\mathrm{w}}$ exists and we have the following two bounds:

$$\left\| \hat{\mathbf{w}}_{|k} - \left(\hat{\mathbb{E}} \left[\frac{\mathbf{x}_{|k} \mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2} \right] \right)^{-1} \hat{\mathbb{E}} \left[\frac{y \mathbf{x}_{|k}}{\|\mathbf{x}_{|d-k}\|^2} \right] \right\|$$

$$\leq \frac{2 \left\| \hat{\mathbb{E}} \left[\frac{y \mathbf{x}_{|k}}{\|\mathbf{x}_{|d-k}\|^2} \right] \right\|}{\lambda_{\min} \left(\hat{\mathbb{E}} \left[\frac{\mathbf{x}_{|k} \mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2} \right] \right)^2} \cdot \frac{1}{m} + \frac{2 \sqrt{\hat{\mathbb{E}}[\|\mathbf{x}_{|k}\|^2] \cdot \hat{\mathbb{E}}[y^2]}}{\min_i \|\mathbf{x}_{i|d-k}\|^4} \cdot m \cdot \|E\|,$$

and

$$\|\hat{\mathbf{w}}_{|d-k}\| \leq \frac{\sqrt{\hat{\mathbb{E}}[\|\mathbf{x}_{|d-k}\|^2] \cdot \hat{\mathbb{E}}[y^2]}}{\min_i \|\mathbf{x}_{i|d-k}\|^2} \cdot \left(1 + \frac{2\|E\|}{\min_i \|\mathbf{x}_{i|d-k}\|^2} \right) \cdot m.$$

Moving to statistical setting

Make sure that the previous bounds are well-defined there. Let $\mathbb{E}_d$ be shorthand for $\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}_d}$. Assumptions:

1. The quantities $\mathbb{E}_d[\|\mathbf{x}\|^4]$, $\mathbb{E}_d[y^4]$, $\mathbb{E}_d[\|y\mathbf{x}_{|k}\|^2/\|\mathbf{x}_{|d-k}\|^4]$, and $\mathbb{E}_d[\|\mathbf{x}_{|k}\|^4/\|\mathbf{x}_{|d-k}\|^4]$ are all bounded in the supremum over d,
2. $\inf_d \lambda_{\text{min}}(\mathbb{E}_d[\mathbf{x}_{|k}\mathbf{x}_{|k}^T/\|\mathbf{x}_{|d-k}\|^2]) > 0$,
3. If $\{\mathbf{x}_i, y_i\}_{i=1}^{m_d}$ are IID samples from $\mathcal{D}_d$, the family $\{\mathbf{x}_i\}_{i=1}^{m_d}$ is linear independent with probability approaching 1,
4. $\min_i \|\mathbf{x}_{i|d-k}\| > c > 0$ with c independent of d,
5. $m_d \cdot \|E\| \xrightarrow{P} 0$, and
6. $m_d^2 \cdot \|\mathbb{E}_d[\mathbf{x}_{|d-k}\mathbf{x}_{|d-k}^T]\| \to 0$.

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Overfitting is generally not benign in regression

Instead of finding the true unique minimizer (benign overfitting)

$$\mathbf{w} = \mathbb{E}_d[\mathbf{x}\mathbf{x}^T]^{-1}\mathbb{E}_d[y\mathbf{x}], \quad \text{i.e.} \quad \mathbf{w}_{|k} = \left(\mathbb{E}_d[\mathbf{x}\mathbf{x}^T]^{-1}\right)_k \mathbb{E}_d[y\mathbf{x}]$$

we find asymptotic behavior of the form

$$\mathbb{E}_d\left[\left(\mathbf{x}^T\hat{\mathbf{w}}_d - \mathbf{x}_{|k}^T\hat{\mathbf{w}}_{d|k}\right)^2\right] \xrightarrow{P} 0, \quad \left\|\hat{\mathbf{w}}_{|k} - \underbrace{\left(\hat{\mathbb{E}}\left[\frac{\mathbf{x}_{|k}\mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2}\right]\right)^{-1}\hat{\mathbb{E}}\left[\frac{y\mathbf{x}_{|k}}{\|\mathbf{x}_{|d-k}\|^2}\right]}\right\| \xrightarrow{P} 0.$$

- Even in ”textbook benign” settings, benign overfitting does not generally occur in misspecified case.

Outline

Trick

Let $\ell_y(\cdot)$ non-negative loss function with unique zero for any y at $\ell_y^{-1}(0)$. Observation:

$$\arg\min_{\mathbf{w}} \|\mathbf{w}\| : \frac{1}{m}\sum_{i=1}^{m} \ell_{y_i}(\mathbf{x}_i^T\mathbf{w}) = 0$$

equals

$$\arg\min_{\mathbf{w}} \|\mathbf{w}\| : \frac{1}{m}\sum_{i=1}^{m} \left(\mathbf{x}_i^T\mathbf{w} - \ell_{y_i}^{-1}(0)\right)^2 = 0$$

Generalized linear model

Suppose $\sigma : \mathbb{R} \to \mathbb{R}$ is a function with Lipschitz inverse and $y = \sigma(\mathbf{x}_{|k}^T \mathbf{w}^*) + \xi$. Then,

$$\mathbb{E}_d\left[(\mathbf{x}^T \hat{\mathbf{w}}_d - \mathbf{x}_{|k}^T \hat{\mathbf{w}}_{d|k})^2\right] \xrightarrow{P} 0, \quad \left\| \hat{\mathbf{w}}_{|k} - \left(\hat{\mathbb{E}}\left[\frac{\mathbf{x}_{|k}\mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2}\right]\right)^{-1} \hat{\mathbb{E}}\left[\frac{\sigma^{-1}(y)\mathbf{x}_{|k}}{\|\mathbf{x}_{|d-k}\|^2}\right] \right\| \xrightarrow{P} 0.$$

- Even in the well-specified case we cannot expect benign overfitting to occur.
- Example: $\|\mathbf{x}_{|d-k}\| = 1$ a.s, $\sigma(0) = 0$, $\mathbf{w}^* = 0$, but $\mathbb{E}[\mathbf{x}_{|k}] \neq 0$, then $\hat{\mathbf{w}}_{|d-k} \approx \left(\mathbb{E}[\mathbf{x}_{|k}\mathbf{x}_{|k}^T]\right)^{-1} \mathbb{E}[\mathbf{x}_{|k}] \cdot \mathbb{E}[\sigma^{-1}(\xi)]$, so necessarily $\mathbb{E}[\sigma^{-1}(\xi)] = 0$ but ...

Lemma

If $\sigma^{-1}(\cdot)$ is such that $\mathbb{E}[\sigma^{-1}(\xi)] = 0$ for all zero-mean RVs ξ with support of size at most 2, then σ (and hence σ^{-1}) must be linear.

Convex losses

Assume $\ell_y(\mathbf{x}^T\mathbf{w}) = f(\mathbf{x}^T\mathbf{w} - y)$ for some non-negative f with unique root at 0 and L_d is defined in terms of this. Then for the min-norm predictor $\hat{\mathbf{w}}$,

$$\mathbb{E}_d\left[(\mathbf{x}^T\hat{\mathbf{w}}_d - \mathbf{x}_{|k}^T\hat{\mathbf{w}}_{d|k})^2\right] \xrightarrow{P} 0, \qquad \left\| \hat{\mathbf{w}}_{|k} - \underbrace{\left(\hat{\mathbb{E}}\left[\frac{\mathbf{x}_{|k}\mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2}\right]\right)^{-1} \hat{\mathbb{E}}\left[\frac{y\mathbf{x}_{|k}}{\|\mathbf{x}_{|d-k}\|^2}\right]} \right\| \xrightarrow{P} 0.$$

- $\hat{\mathbf{w}}_{|k}$ has same asymptotic characterization as before
- we can't expect this to be optimal for the objective $\mathbb{E}[f(\mathbf{x}^T\mathbf{w} - y)]$

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Implicit bias towards weighted square loss problem

We found asymptotically

$$\hat{\mathbf{w}}_{d|k} \approx \left(\hat{\mathbb{E}}\left[\frac{\mathbf{x}_{|k}\mathbf{x}_{|k}^T}{\|\mathbf{x}_{|d-k}\|^2}\right]\right)^{-1}\hat{\mathbb{E}}\left[\frac{y\mathbf{x}_{|k}}{\|\mathbf{x}_{|d-k}\|^2}\right]$$

Thus, the first k coordinates actually optimize the objective function

$$\mathbb{E}_d\left[\left(\frac{\mathbf{x}^T}{\|\mathbf{x}_{|d-k}\|}\mathbf{w} - \frac{y}{\|\mathbf{x}_{i|d-k}\|}\right)^2\right]$$

- $\hat{\mathrm{w}}$ is consistent w.r.t. the statistical problem that is using the empirical version of the above as loss.

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Max-margin classifier

- Now consider RVs $(\mathbf{x}, y) \sim \mathbb{R}^d \times \{-1, 1\}$
- Same conventions for the sequence $\{\mathcal{D}_d\}_{d=k+1}^{\infty}$ of distributions as before
- Now, true risk $R_d = \Pr_{(\mathbf{x},y)}\{y\mathbf{x}^T\mathbf{w} \leq 0\}$
- Standard gradient methods run on standard convex classification loss (e.g. logistic or cross-entropy) converge in direction of the max-margin predictor

$$\hat{\mathbf{w}} := \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{w}\| : \ \min_i y_i \mathbf{x}_i^T \mathbf{w} \geq 1$$

Benign overfitting

A sequence of distributions $\{\mathcal{D}_d\}_{d=k+1}^{\infty}$ satisfies benign overfitting if there is a sequence of sample sizes $\{m_d\}_{d=k+1}^{\infty}$ such that

- $\hat{\mathbf{w}}_d$ exists with probability approaching 1,
- $\inf_d \inf_{\mathbf{w}\in\mathbb{R}^d} R_d(\mathbf{w}) > 0$, and
- $R_d(\hat{\mathbf{w}}_d) - \inf_{\mathbf{w}\in\mathbb{R}^d} R_d(\mathbf{w}) \xrightarrow{P} 0$

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Deterministic perturbation bound

Let $\{(\mathbf{x}_i, y_i\}_{i=1}^m$ be a deterministic sample of size m. Define the perturbation matrix

$$E_{ij} := y_i y_j \mathbf{x}_{i|d-k}^T \mathbf{x}_{j|d-k} \cdot \mathbf{1}\{i \neq j\} \in \mathbb{R}^{m \times m}.$$

Assume that the max-margin predictor exists and suppose

$$\epsilon_0 := \frac{2\|E\| \cdot \max_i \|\mathbf{x}_{i|d-k}\|^2}{\min_i \|\mathbf{x}_{i|d-k}\|^4} \leq \frac{1}{2}.$$

Then,

$$\hat{\mathbf{w}}_{|k} = \arg\min_{\mathbf{v} \in \mathbb{R}^k} (1 + \epsilon_{\mathbf{v}}) \cdot \hat{\mathbb{E}} \left[\frac{[1 - y\mathbf{x}_{|k}^T \mathbf{v}]_+^2}{\|\mathbf{x}_{|d-k}\|^2} \right] + \frac{\|\mathbf{v}\|^2}{m} \quad \text{with } \sup_{\mathbf{v}} |\epsilon_{\mathbf{v}}| \leq \epsilon_0,$$

and

$$\|\mathbf{w}_{|d-k}\|^2 \leq \frac{5m}{\min_i \|\mathbf{x}_{i|d-k}\|^2}.$$

Moving to statistical setting

Assumptions:

1. $\sup_d \mathbb{E}_d \left[\frac{1+\|y\mathbf{x}_k\|^4}{\|\mathbf{x}_{|d-k}\|^4}\right] < \infty$,
2. With probability approaching 1 (as $d \to \infty$), the max-margin predictor $\hat{\mathrm{w}}_d$ exists and $0 > c \geq \max_i \max\{\|\mathbf{x}_{i|d-k}\|^{-1}, \|\mathbf{x}_{i|d-k}\|\}$,
3. $m_d \cdot \|E\| \xrightarrow{P} 0$,
4. $m_d \cdot \|\mathbb{E}_d[\mathbf{x}_{|d-k}\mathbf{x}_{|d-k}^T]\| \to 0$.

Setting

$$g_d(\mathbf{v}) := \mathbb{E}_d \left[\frac{[1 - y\mathbf{x}_{|k}^T\mathbf{v}]_+^2}{\|\mathbf{x}_{|d-k}\|^2}\right], \quad \text{and} \quad \hat{g}_d(\mathbf{v}) := \hat{\mathbb{E}}_d \left[\frac{[1 - y\mathbf{x}_{|k}^T\mathbf{v}]_+^2}{\|\mathbf{x}_{|d-k}\|^2}\right].$$

5. There exists $c' > 0$ independent of d such that with probability approaching 1, $\hat{g}_d$ has a minimizer of norm at most c',
6. $\inf_{\mathbf{v}} \limsup_d \left(g_d(\mathbf{v}) - \inf_{\mathbf{u}} g_d(\mathbf{u})\right) = 0$.

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Asymptotic characterization of max-margin predictor

Under these assumptions, with

$$g_d(\mathbf{v}) := \mathbb{E}_d\left[\frac{[1 - y\mathbf{x}_{|k}^T\mathbf{v}]_+^2}{\|\mathbf{x}_{|d-k}\|^2}\right], \quad \text{and} \quad \hat{\mathbf{w}}_d = \arg\min_{\mathbf{w}} \|\mathbf{w}\| : \ \min_i y_i \mathbf{x}_i^T \mathbf{w} \geq 1,$$

the max-margin predictor satisfies

$$g_d(\hat{\mathbf{w}}_{d|k}) - \inf_{\mathbf{v}} g_d(\mathbf{v}) \xrightarrow{P} 0, \quad \text{and} \quad \mathbb{E}_d\left[(\mathbf{x}^T\hat{\mathbf{w}}_d - \mathbf{x}_{|k}^T\hat{\mathbf{w}}_{d|k})^2\right] \xrightarrow{P} 0.$$

- The junk features are asymptotically negligible, and the relevant ones actually minimize a scaled squared hinge loss.
- Whether minimizers of g_d also have small misclassification error is equivalent to asking whether this weighted squared hinge loss is a good surrogate.

Study setting

The characterization makes the following assumptions look mild:

1. The joint distribution of $(\mathbf{x}_{|k}, \|\mathbf{x}_{|d-k}\|, y)$ is the same under any d,
2. $\mathbb{E}[\mathbf{x}_{|k}\mathbf{x}_{|k}^T]$ is positive definite
3. $\Pr\{\|\mathbf{x}_{|d-k}\| \in I\} = 1$ for a closed interval $I \subset (0, \infty)$.

Let $(\mathbf{x}_{|k}, y)$ be distributed according to a linearly separable distribution $\mathcal{D}_{\text{clean}}$ but implement label flips via the loss function:

$$L_p(\mathbf{w}) := \mathbb{E}_{(\mathbf{x}_{|k}, z, y) \sim \mathcal{D}_{\text{clean}}}[z \cdot \ell_p(y\mathbf{x}_{|k}^T\mathbf{w})], \quad \text{where} \quad \ell_p(\beta) := (1-p) \cdot [1-\beta]_+^2 + p \cdot [1+\beta]_+^{-1}$$

- for $p \in (0, \frac{1}{2})$, L_p is strongly convex $\implies$ unique minimizer $\mathbf{w}_p^*$
- benign overfitting happens if $\Pr_{(\mathbf{x}_{|k}, y) \sim \mathcal{D}_{\text{clean}}}\{y\mathbf{x}_{|k}^T\mathbf{w}_p^* \le 0\} = 0$

Classification setting favorable for benign overfitting

Two cases in which we have benign overfitting

Theorem

$(\mathbf{x}_{|k}, z, y) \sim \mathcal{D}_{\text{clean}}$ any distribution so that $(\mathbf{x}_{|k}, y)$ linearly separable and $\mathbf{x}_{|k}$ has bounded support. Then, there is $a \in (0, \frac{1}{2}$ dependent on $\mathcal{D}_{\text{clean}}$ such that for all $p \in (0, a)$ we have

$$\Pr_{(\mathbf{x}_{|k}, y) \sim \mathcal{D}_{\text{clean}}} \{y \mathbf{x}_{|k}^T \mathbf{w}_p^* \leq 0\} = 0.$$

Theorem

$(\mathbf{x}_{|k}, z, y) \sim \mathcal{D}_{\text{clean}}$ any distribution so that $(\mathbf{x}_{|k}, y)$ linearly separable. Suppose that for some unit vector $\mathbf{u}$ and conditioned on any value of y,

- $\mathbf{u}^T \mathbf{x}$ and $(I - \mathbf{u}\mathbf{u}^T)\mathbf{x}$ are mutually independent, and
- the distributions of $(I - \mathbf{u}\mathbf{u}^T)\mathbf{x}$ and $-(I - \mathbf{u}\mathbf{u}^T)\mathbf{x}$ are identical.

Then, for all $p \in (0, \frac{1}{2})$ we have

$$\Pr_{(\mathbf{x}_{|k}, y) \sim \mathcal{D}_{\text{clean}}} \{y \mathbf{x}_{|k}^T \mathbf{w}_p^* \leq 0\} = 0.$$