

# Policy Learning in High Dimensional Settings

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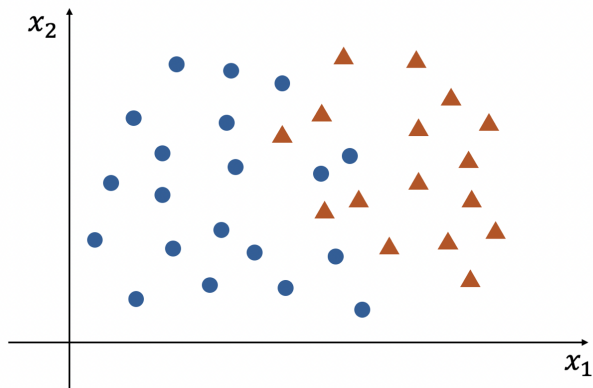
Brown University

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# Overview

- 1 Classification
- 2 Weighted Classification and Policy Learning
- 3 Policy Learning in High Dimension
- 4 Weighted Generalization Bounds
- 5 Discussions

# Classification Problem



- A sample  $\{X_i, t_i\}_{i=1}^n$  drawn from distribution  $P$  over  $\mathcal{X} \times \{+1, -1\}$ .
- Want to learn a function  $g$  that maps from  $\mathcal{X}$  to  $\{+1, -1\}$  to minimize risk.

# Population and Empirical Risk

- Population risk or classification risk of a function  $g$ :

$$R(f) = E_P[\mathbf{1}\{t_i g(\mathbf{x}) < 0\}]$$

- Empirical risk or sample risk of a function  $g$ :

$$\hat{R}(f) = \frac{1}{m} \sum_{i=1}^m \mathbf{1}\{t_i g(\mathbf{x}_i) < 0\}$$

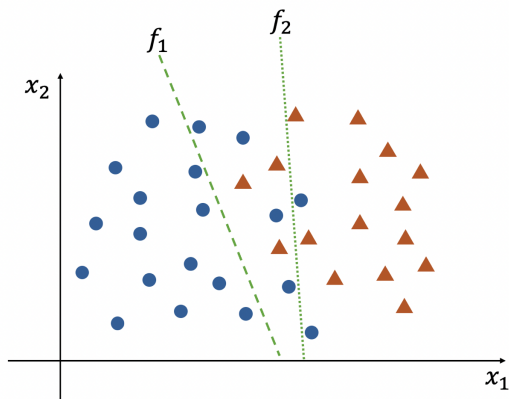
- Every binary classifier  $g$  can be written as:

$$g = \text{sign}(f(\mathbf{x}_i))$$

where  $f(\mathbf{x}_i)$  is a real valued function.

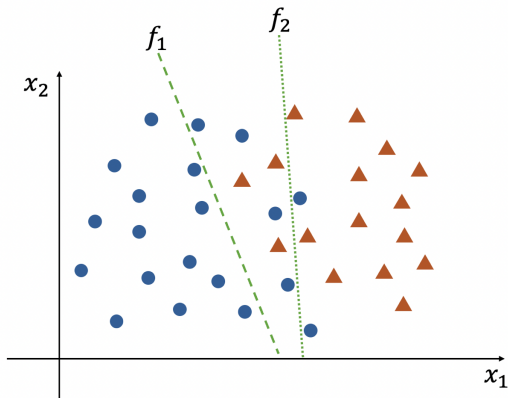
- Examples of  $f$  can be linear function, neural network etc.

# How to Learn $f$ ?



- Empirical risk minimization (ERM) principle: fix a hypothesis class e.g. the class of all linear functions.
- Choose the function in the hypothesis class that minimizes empirical risk.

# How to Learn $f$ ?



- 20 circle, 16 triangles in the sample.
- $f_1$  has risk  $\frac{6}{36}$ ,  $f_2$  has risk  $\frac{5}{36}$ . ERM would pick  $f_2$  over  $f_1$ .

# Surrogate Loss and Optimization

- Fixing a hypothesis class, minimizing  $\hat{R}(f)$  directly is not tractable most of the times.
- Minimize surrogate risk instead:

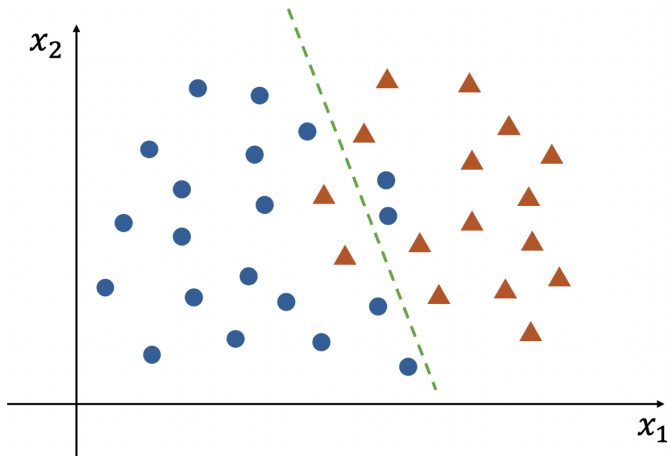
$$\hat{R}_\phi(f) = \frac{1}{m} \sum_{i=1}^m \phi(t_i f(\mathbf{x}_i))$$

- Examples of  $\phi$  can be  $\phi(\alpha) = \max\{0, 1 - \alpha\}$ .
- Numerical optimization such as gradient descent.
- Please refer to Kitagawa et al (2023) for a comprehensive treatment of this topic.

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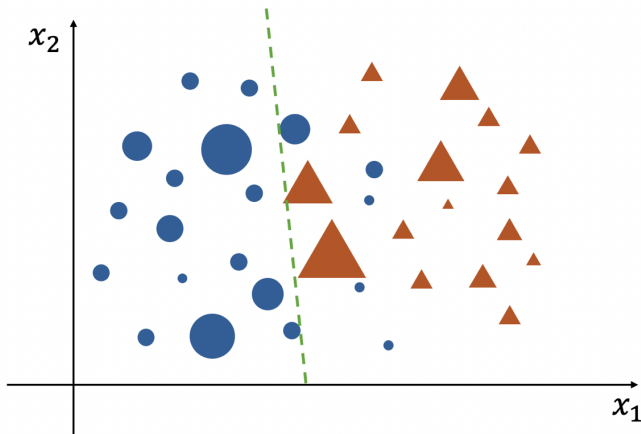
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# Unweighted Classification



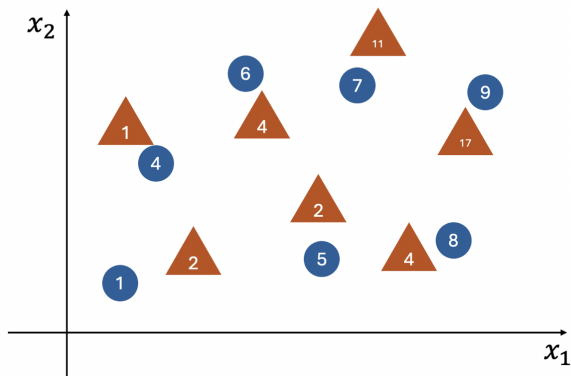
- Decision boundary for an unweighted classification problem.

# Weighted Classification



- Decision boundary for an weighted classification problem.
- Weighted empirical risk:  $\hat{R}^\omega(f) = \frac{1}{m} \sum_{i=1}^m \omega_i \mathbf{1}\{t_i \text{sign}(f(\mathbf{x}_i)) < 0\}$ .

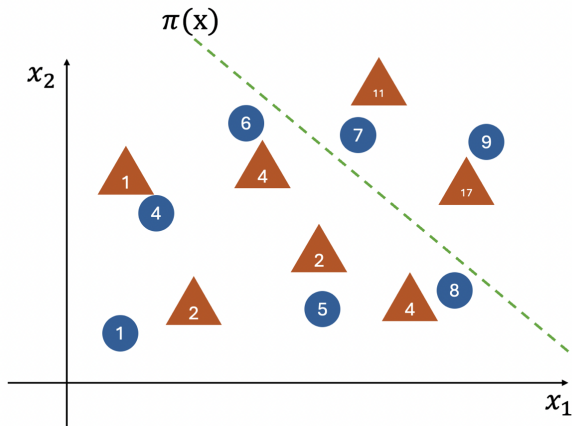
# Policy Learning



- A sample  $\{X_i, D_i, Y_i\}_{i=1}^m$  drawn from distribution  $Q$ .
- Want to learn a function  $\pi$  that maps from  $\mathcal{X}$  to  $\{+1, -1\}$  to maximize population welfare.

$$W(f) := E_Q[y_i(+1)\mathbf{1}\{f(\mathbf{x}_i) \geq 0\} + y_i(-1)\mathbf{1}\{f(\mathbf{x}_i) < 0\}]$$

# Policy Learning Intuition



- Example of a treatment assignment rule.
- Oracle policy is to assign treatment according to  $CATE(\mathbf{x}_i) \geq 0$ .

# Classification and Policy Learning

## Proposition (Risk minimization and welfare maximization (Kitagawa et al (2023)))

Assuming  $e(x)$  and  $Q$  satisfy the following properties:

- *Overlap: propensity score*  $0 < e(x) < 1$  for all  $x \in \mathcal{X}$
- *Unconfoundedness:*  $y_i(+1), y_i(-1) \perp D_i | \mathbf{x}_i$

Then the maximization of additive welfare criterion  $W(f)$  is equivalent to the minimization of weighted classification risk

$$E_Q[\omega_i \mathbf{1}\{t_i \text{sign}(f(\mathbf{x}_i)) < 0\}]$$

where  $t_i = \text{sign}(y_i)D_i$  and  $\omega_i = \frac{|y_i|}{D_i e(\mathbf{x}_i) + (1 - D_i)/2}$ .

- $W(f) := E_Q[y_i(+1)\mathbf{1}\{f(\mathbf{x}_i) \geq 0\} + y_i(-1)\mathbf{1}\{f(\mathbf{x}_i) < 0\}]$

# Classification and Policy Learning

- If a unit has large observed outcome, then it is valuable for the model to match the treatment status  $D_i$  of the unit because mismatching  $\text{sign}(f(\mathbf{x}_i))$  and  $D_i$  is costly.
- Population welfare in terms of conditional average treatment effect  $\tau(\mathbf{x}_i)$ :

$$W(f) = E_Q[y_i(-1)] + E_Q[\mathbf{1}\{\text{sign}(f(\mathbf{x}_i)) \geq 0\}\tau(\mathbf{x}_i)]$$

- The weighted classification boundary is in fact the CATE threshold at 0.
- What happens if we conduct policy learning with high dimensional features but limited sample size?

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# Contributions

- Demonstrated that by doing policy learning via weighted classification, “double ascent” phenomenon of welfare exists in overparameterized / high dimensional settings.
- Using a rich set of features and highly overparameterized models might lead to higher welfare than using a restricted model.

# Contributions

- Extended existing results on generalization bounds to weighted classification and additive welfare maximization.
- Explained the “double ascent” phenomena via the above generalization bounds by building on Lee & Cherkassky (2024).
- Suggestions for practitioners: potential value of flexible, high dimensional policy rules using rich covariate information.

# Data Generating Process

We use the following RCT data generation set-up.  $n$  units  $\{\mathbf{x}_i, D_i, y_i(+1), y_i(-1)\}_{i=1}^m$  are randomly drawn from:

$$\mathbf{x}_i \sim N_d(0, \sigma_x^2 I_d) \quad (1)$$

$$y_i(+1) = \mathbf{x}_i^T \beta_1 + \epsilon_{1,i} \quad (2)$$

$$y_i(-1) = \mathbf{x}_i^T \beta_0 + \epsilon_{0,i} \quad (3)$$

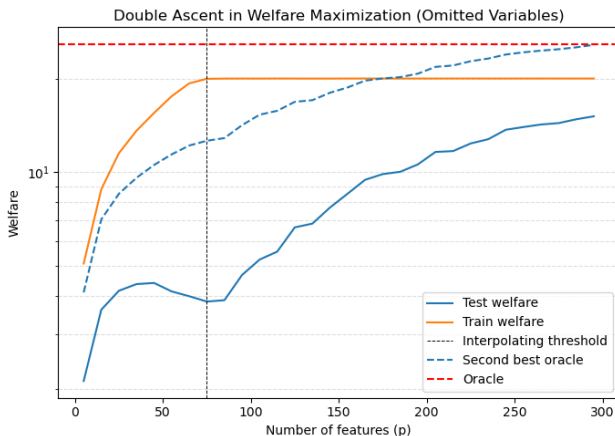
$$D_i \sim \text{symmetric Bernoulli}(q) \quad (4)$$

- Potential outcomes are not observed. We observe a sample  $\{\mathbf{x}_i, D_i, y_i\}_{i=1}^m$ , where  $y_i = (\frac{1+D_i}{2}) \cdot y_i(+1) + (\frac{1-D_i}{2}) \cdot y_i(-1)$ .
- $CATE(\mathbf{x}_i) = \mathbf{x}_i^T (\beta_1 - \beta_0)$ .
- $\epsilon_{1,i}$  and  $\epsilon_{0,i}$  have zero mean.

# Omitted Variables

- Sample size  $m$  fixed at 150.  $\mathbf{x}_i \in \mathbb{R}^{300}$ .
- For  $p \in [5, 10, \dots, 300]$ :
  - Take the first  $p$  features of  $\mathbf{x}_i$ , denote it by  $\tilde{\mathbf{x}}_{ip}$ .
  - Fit  $g(\tilde{\mathbf{x}}_{ip}) = \text{sign}(\tilde{\mathbf{x}}_{ip}^T \alpha_p)$  by optimizing  $\mathcal{L}(\alpha_p) = \frac{1}{m} \sum_{i=1}^m \omega_i \phi(t_i \tilde{\mathbf{x}}_{ip}^T \alpha_p)$  using gradient descent, where  $\phi(c) = \log(1 + e^{-c})$  logistic loss.
  - Signal strength increases linearly in  $\beta_1$  and  $\beta_0$ , though this can be relaxed and obtain qualitatively similar results.
- Repeat the above and average over 200 runs.

# Omitted Variables results

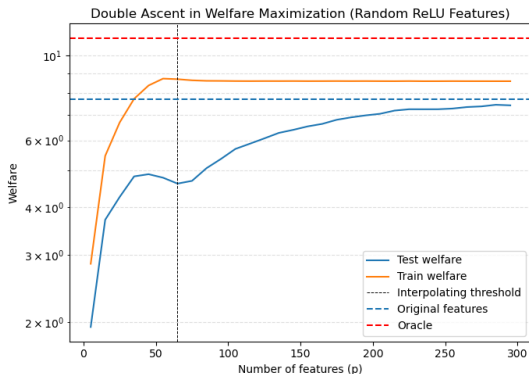


- Gap between the two oracles due to omitted variables.
- Gap between second best oracle and test welfare due to sampling error and using surrogate loss.
- Second ascent in welfare despite heavily overparameterized.

# Random Features

- Sample size  $m$  fixed at 150.  $\mathbf{x}_i \in \mathbb{R}^{50}$ .
- Instead of observing  $\mathbf{x}_i$ , for  $p \in [5, 10, \dots, 300]$ ,:
  - We observe  $\mathbf{z}_i = \sigma(W_p \mathbf{x}_i)$  where  $W_p \in \mathbb{R}^{p \times 50}$  is a random matrix drawn from multivariate normal.  $\sigma(\cdot)$  is a nonlinear activation function.
  - Fit  $g(\mathbf{z}_i) = \text{sign}(\mathbf{z}_i^T \alpha_p)$  by optimizing  $\mathcal{L}(\alpha_p) = \frac{1}{m} \sum_{i=1}^m \omega_i \phi(t_i \mathbf{z}_i^T \alpha_p)$  using gradient descent, where  $\phi(c) = \log(1 + e^{-c})$  logistic loss.
- Repeat and average over 200 runs.
- Akin to observing noisy measures of a set of lower dimensional true features.

# Random Feature Results



- Gap between oracle and using original features due to sampling error.
- Gap between original features and test welfare due to surrogate loss and parameterization.
- Regardless of the dimension of  $\mathbf{x}_i$ , test welfare converges to original features as  $p/n$  increases.

# Other Simulations

“Double ascent” is also observed when:

- True CATE is nonlinear in  $\mathbf{x}_i$  but we fit the same linear treatment assignment rule.
- True CATE is linear in  $\mathbf{x}_i$  and for each value of  $p$ , the true DGP has the same feature dimensions as the observed sample, i.e. “moving target”.

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# Quantifying Complexities

- Empirical Rademacher Complexity of a set of bounded real valued functions  $\mathcal{G}$ , fixing a sample  $S$ :

$$\hat{\mathfrak{R}}_S(\mathcal{G}) := E_\sigma \left[ \sup_{g \in \mathcal{G}} \frac{1}{m} \sum_{i=1}^m \sigma_i g(x_i) \right] = E_\sigma \left[ \sup_{g \in \mathcal{G}} \frac{1}{m} \sigma \cdot \mathbf{g} \right]$$

- How well the functions in  $\mathcal{G}$  can fit random noise on average.

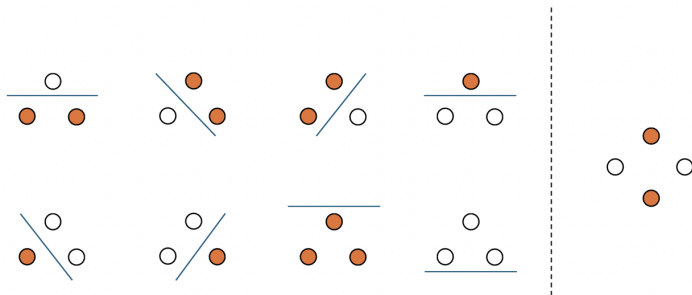
# Quantifying Complexities

- VC dimension of a set of binary functions  $\mathcal{G}$  is the size of the largest set that can be shattered by  $\mathcal{G}$ :

$$VCdim(\mathcal{G}) = \max\{m : \Pi_{\mathcal{G}}(m) = 2^m\}$$

where  $\Pi_{\mathcal{G}}(m)$  is the maximum number of distinct ways in which  $m$  points can be classified using hypothesis in  $\mathcal{G}$ .

# VC Dimension example



The VC dimension of a hyperplane in  $\mathbb{R}^n$  is  $n + 1$ .

# Bounded Weights

## Proposition (VC-dimension generalization bound for weighted classification)

Let  $\mathcal{H}$  be a class of functions taking values in  $\{+1, -1\}$  with VC-dimension  $d$ . Assume that the classification weight  $\omega$  is bounded between  $0 \leq \omega \leq W$  where  $W = \sup \omega$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$  over a sample  $S$  of size  $m$ , the following holds for all  $f \in \mathcal{H}$ :

$$R^\omega(f) \leq \hat{R}^\omega(f) + W \left( \sqrt{\frac{2d \log \frac{em}{d}}{m}} + \sqrt{\frac{\log \frac{1}{\delta}}{2m}} \right) \quad (5)$$

$$= O \left( W \sqrt{\frac{\log \frac{m}{d}}{\frac{m}{d}}} \right) \quad (6)$$

where  $m$  is the size of the training sample.

# Proof Sketch

- Uniformly bound the empirical process  $R^\omega(f) - \hat{R}^\omega(f)$  using McDiarmid's Inequality in terms of Rademacher complexity.
- Then bound Rademacher complexity with VC dimension.

# Sub-gaussian Weights

## Proposition (VC-dimension generalization bound with sub-Gaussian weights)

Let  $\mathcal{H}$  be a class of functions taking values in  $\{+1, -1\}$  with VC-dimension  $d$ . Assume that the classification weight  $\omega$  is sub-Gaussian with constant  $K$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$  over a sample  $S$  of size  $m$ , the following holds for all  $f \in \mathcal{H}$ :

$$R^\omega(f) \leq \hat{R}^\omega(f) + K \sqrt{\log \frac{2m}{\delta}} \left( 2\sqrt{\frac{d \log \frac{em}{d}}{m}} + \sqrt{\frac{\log \frac{2}{\delta}}{m}} \right) \quad (7)$$

$$= O \left( \sqrt{\log m} \sqrt{\frac{\log \frac{m}{d}}{\frac{m}{d}}} \right) \quad (8)$$

where  $m$  is the size of the training sample.

# Welfare Generalization Bound

## Corollary (VC-dimension generalization bound for welfare)

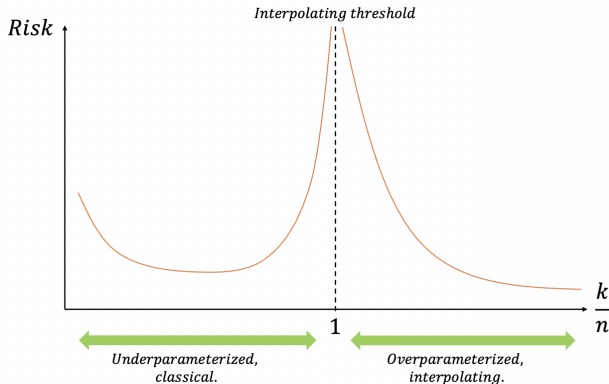
Let  $\mathcal{H}$  be a class of functions taking values in  $\{+1, -1\}$  with VC-dimension  $d$ . Suppose that the population distribution is  $Q$ , and that the classification weight, which is defined as  $\omega := \frac{|y_i|}{D_i e(\mathbf{x}_i) + (1 - D_i)/2}$ , is sub-Gaussian with constant  $K$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$  over a sample  $S$  of size  $m$ , the following holds for all  $f \in \mathcal{H}$ :

$$W(f) \geq \hat{W}(f) - K \sqrt{\log \frac{2m}{\delta}} \left( 2 \sqrt{\frac{d \log \frac{em}{d}}{m}} + \sqrt{\frac{\log \frac{2}{\delta}}{m}} \right) + C_{Q,m} \quad (9)$$

where  $m$  is the size of the training sample,  $C_{Q,m}$  is a constant that depends only the population distribution  $Q$  and the random sample and is independent of  $f$ , and empirical welfare as a function of treatment assignment rule  $f$  is defined as

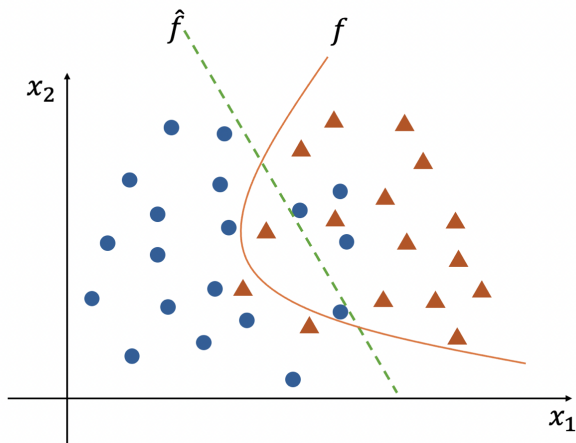
$$\hat{W}(f) = \frac{1}{n} \sum_{i=1}^n (y_i(+1) \mathbf{1}\{f(\mathbf{x}_i) \geq 0\} + y_i(-1) \mathbf{1}\{f(\mathbf{x}_i) < 0\}).$$

# Underparameterized Regime



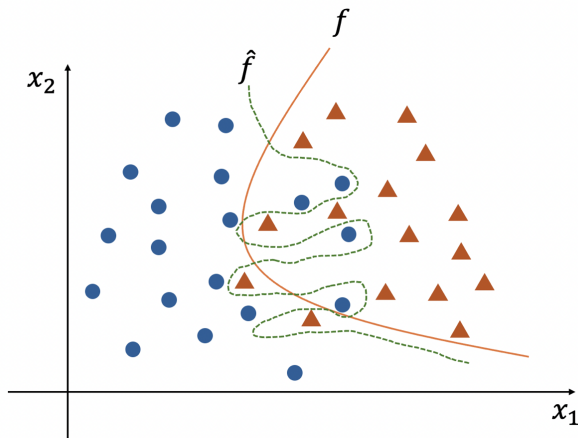
- The usual tradeoff between bias and variance.
- The drop in population risk with decrease in empirical risk is counterbalanced by the increase in model (hypothesis class) complexity.

# Underparameterized Regime



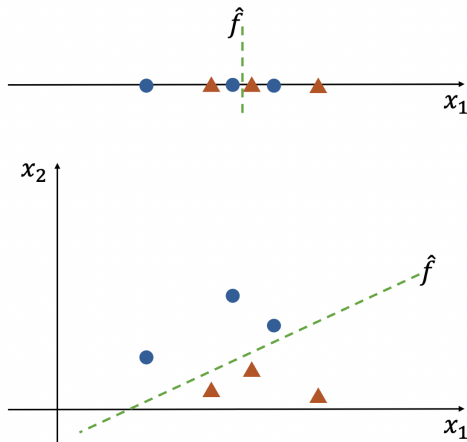
- High bias due to low complexity of the hypothesis class.

# Underparameterized Regime



- High variance due to high complexity of the hypothesis class.

# Overparameterized Regime Intuition



- Adding more dimensions gives the classifier higher flexibility to separate data. Hypothesis class becomes richer.
- Binary classification problem becomes linearly separable in higher dimensions.

# Overparameterized regime

- However, in overparameterized regime, classifiers often have no unique solution to minimizing empirical loss.
- The loss function has many global minima i.e. loss equals 0. Most of them do not generalize well.
- Optimization algorithm matters! Certain algorithms have implicit bias that lead to a global minimum that generalizes well. E.g. gradient descent with squared loss in overparameterized linear regression leads to the ridgeless interpolator.
- Soudry et al (2018) show that in usual classification, linear classifier with gradient descent converges to the maximum hyperplane for linearly separable data.

# Convergence to SVM

## Proposition (Convergence to SVM with Weighted Loss)

*For any dataset that is linearly separable, suppose surrogate loss function  $\phi$  and learning rate  $\eta$  satisfy the conditions in Theorem 3 of Soudry et al (2018). For a linear classifier  $f(\mathbf{x}_i) = \mathbf{x}_i^T \mathbf{w}$ , let  $\mathbf{w}(t)$  be the weight at iteration  $t$  of gradient descent, for both*

$$\mathcal{L}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^m \phi(t_i \text{sign}(\mathbf{x}_i^T \mathbf{w})) \text{ and}$$

$$\mathcal{L}^\omega(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^m \omega_i \phi(t_i \text{sign}(\mathbf{x}_i^T \mathbf{w})), \text{ the following holds:}$$

$$\lim_{t \rightarrow \infty} \frac{\mathbf{w}(t)}{\|\mathbf{w}(t)\|} = \frac{\hat{\mathbf{w}}}{\|\hat{\mathbf{w}}\|} \quad (10)$$

*for almost all datasets (all except measure zero) and strictly positive  $\omega_j$ .  $\hat{\mathbf{w}}$  is the direction of the max-margin SVM*

# Convergence to SVM Intuition

- Gradient flow:

$$-\nabla \mathcal{L}(\mathbf{w}(t)) = \sum_{i=1}^m \omega_i \exp(-g(t) \mathbf{w}_\infty^T \mathbf{x}_i y_i) \cdot \exp(-\rho(t)^T \mathbf{x}_n y_i) \mathbf{x}_n y_i$$

- When data is separable,  $g(t) \rightarrow \infty$ ,  $\frac{\rho(t)}{g(t)} \rightarrow 0$ , so only those samples with the largest exponents e.g. smallest  $g(t) \mathbf{w}_\infty^T \mathbf{x}_i y_i$  will contribute to the gradient, i.e. the support vectors.
- Max margin SVM solves  $\min \|\mathbf{w}\|^2$  s.t.  $\mathbf{w}^T \mathbf{x}_i y_i \geq 1 \forall i$ . Weighted loss is like replicating the constraints, which does not change the support vectors.

# VC Dimension Bound for SVM

- Vapnik (2000) Theorem 5.1, let  $d$  be the VC dimension of a max margin hyperplane:

$$d \leq \min\left\{\frac{R^2}{\rho^2}, n\right\} + 1$$

where  $\mathbf{x}_i$  is assumed bounded in a sphere of radius  $R$ ,  $\rho$  is the margin of the SVM, and  $n$  is the dimension of the space.

- For max margin SVM:

$$\rho^2 = \frac{1}{\|\hat{\mathbf{w}}\|^2}$$

# Decreasing Complexity in Overparameterized Regime

In the overparameterized regime, empirical welfare is maxed out, so population welfare can be written as:

$$W(f) \approx C - O\left(\sqrt{\log m} \left(\sqrt{\frac{1 + \log \frac{m}{\|\hat{\mathbf{w}}\|^2}}{\frac{m}{\|\hat{\mathbf{w}}\|^2}}}\right)\right)$$

# Decreasing Complexity

- For max margin SVM,  $\|\hat{\mathbf{w}}\|$  is non-increasing in the dimension of  $\mathbf{x}_i$ , otherwise the additional dimension can have coefficient 0 in the minimization problem.

- In the domain where  $\|\hat{\mathbf{w}}\| \leq \sqrt{m}$ ,  $\sqrt{\frac{1 + \log \frac{m}{\|\hat{\mathbf{w}}\|^2}}{\frac{m}{\|\hat{\mathbf{w}}\|^2}}}$  is strictly decreasing in  $\frac{m}{\|\hat{\mathbf{w}}\|^2}$ .

- First ascent due to bias variance trade-off, second ascent entirely due to complexity control without explicit regularization.
- Relevant explanations: Belkin et al (2020), Deng et al (2020), Kini and Thrampoulidis (2020), Hastie et al (2022).

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# Takeaway for Practitioners

- In certain situations, e.g. you believe the true DGP is high dimensional or a low dimensional set of latent features gives many noisy measurements, practitioners may benefit from overparameterized models because richer feature sets can lead to higher welfare level than more parsimonious specifications.
- Besides linear model with gradient descent, can also consider neural network classifiers. Although shown to work well in practice, theoretical reasons for generalization of NN is an open question.

# Some Complications

- Interpretability.
- Equity.
- Preference for simple decision rules.
- Resource constraints in collecting features.

# Unanswered Questions

- What if using observational data? How does estimating propensity score affect welfare performance?
- How does this compare to existing policy learning methods e.g. Empirical Welfare Maximization, Athey & Wager (2021).
- How does this compare to estimating CATE then plug in CATE for treatment assignment? e.g. deep neural network results of Farrell et al (2021).

Thank you.