DS-GA 1003: Machine Learning

Lecture 3: Regularization and Loss Functions

Slides adapted from material from David Rosenberg.

Logistics & Announcements

* PROJECT: Instructions out soon (within the week)

PS 1 due today! Due 11:59 PM ET, late deadline is Thursday, 11:59 PM ET.

PS 2 release. Due in two weeks, Tuesday, Feb. 17 11:59 PM ET.

Looks long! But most of the problems are review/exposition and subproblems are short.

Lab this week. Sam will be doing lab this week to lighten up the load for next lecture.

Lecture for Week 5 (02/17) is cancelled due to President's Day.

Lecture on Week 6 (02/24) will be remote and recorded. Sam out of town for conference :(

Math review videos. Stay tuned for several linear algebra review videos!

Outline

Excess Risk

Full Decomposition

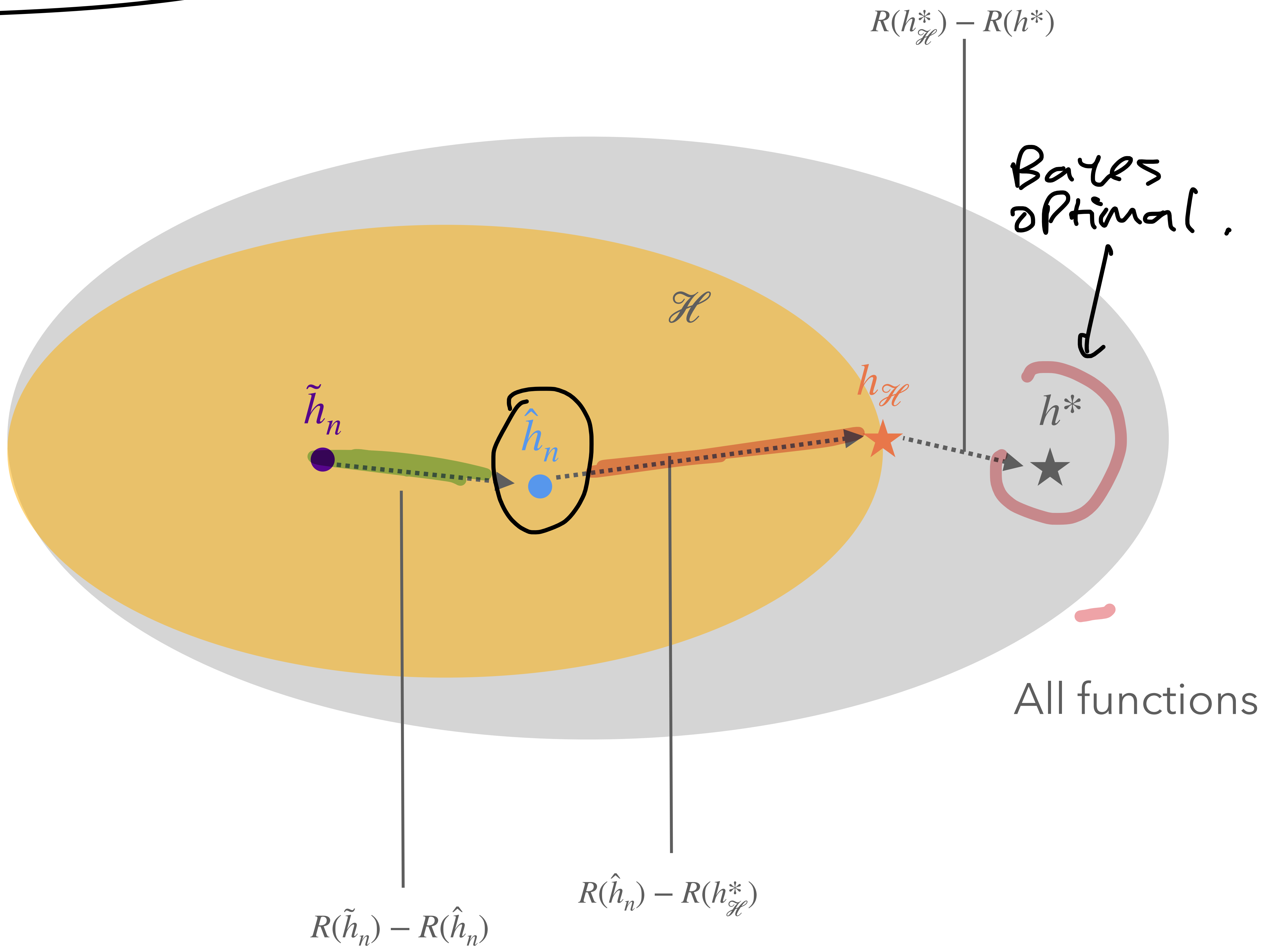
$$\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), y_i)$$

We receive $\tilde{h}_n$ from an algorithm.

Excess risk of $\tilde{h}_n$:

$$R(\tilde{h}_n) - R(h^*) =$$

$$\boxed{\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathcal{H}}) - R(h^*)}_{\text{approx. error}}$$



$R(h^*_{\mathcal{H}}) - R(h^*)$
Bayes optimal.
$\mathcal{H}$
$h_{\mathcal{H}}$
$\tilde{h}_n$
$\hat{h}_n$
h^*
All functions
$R(\tilde{h}_n) - R(\hat{h}_n)$
$R(\hat{h}_n) - R(h^*_{\mathcal{H}})$

Estimation-Approximation Tradeoff

$R(h) = \mathbb{E}[\ell(h(x), y)]$.

Recurring Theme

$\hat{h}_n \in \underset{h \in \mathcal{H}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \underline{\ell(h(x_i), y_i)}$

$R(h) = \underline{\mathbb{E}[\ell(h(x), y)]}$

$$\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(\underline{h^*_{\mathcal{H}}}) - R(\underline{h^*})}_{\text{approx. error}}$$

Estimation error: As $n \to \infty$, typically $R(\hat{h}_n) - R(\underline{h^*_{\mathcal{H}}}) \to 0$.

Approximation error: Controlled by choosing a good hypothesis class $\mathcal{H}$.

Optimization error: Can we make this small using an efficient algorithm?

How does choosing the "size"/"complexity" of $\mathcal{H}$ affect estimation and approximation error?

Supervised Learning

Excess Risk Formalization

1. Collect training dataset, a collection of labeled input-output pairs.

2. Decide on the template of the hypothesis mapping that will map inputs to outputs. Representation

3. A learning algorithm takes the labeled training data as input and outputs a hypothesis. Optimization

4. The hypothesis predicts on new, unseen data which we hope it does well on, under a notion of loss. Generalization

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Optimization Generalization Representation

Supervised Learning

Excess Risk Formalization

1. Collect training dataset, a collection of labeled input-output pairs.

2. Decide on the template of the hypothesis mapping that will map inputs to outputs. — Representation

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$$R(\tilde{h}_n) - R(h^*) =$$

$$\underbrace{R(\tilde{h}_n) - R(\hat{h}_n)}_{\text{opt. error}} + \underbrace{R(\hat{h}_n) - R(h^*_{\mathcal{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathcal{H}}) - R(h^*)}_{\text{approx. error}}$$

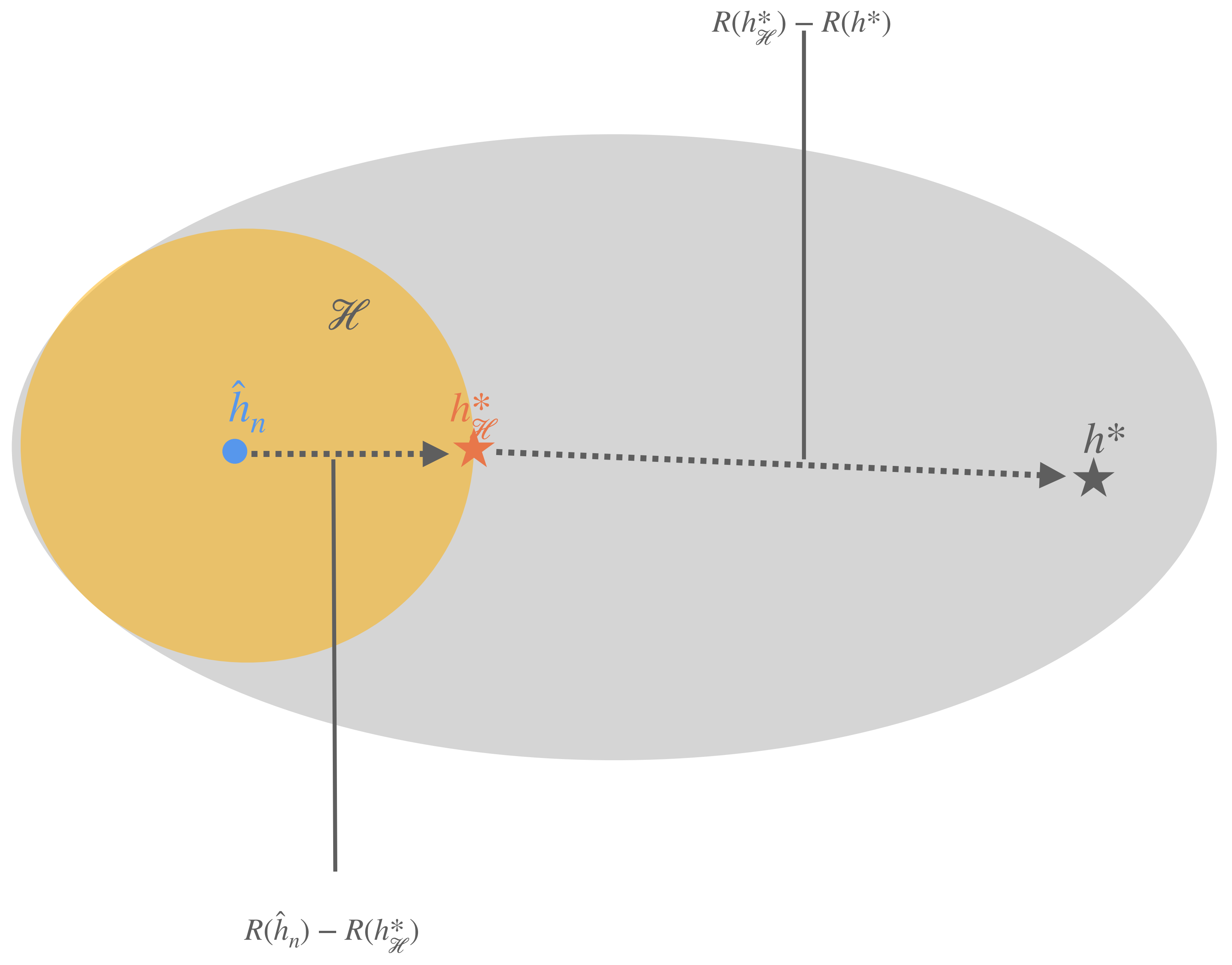
Optimization — Generalization — Representation

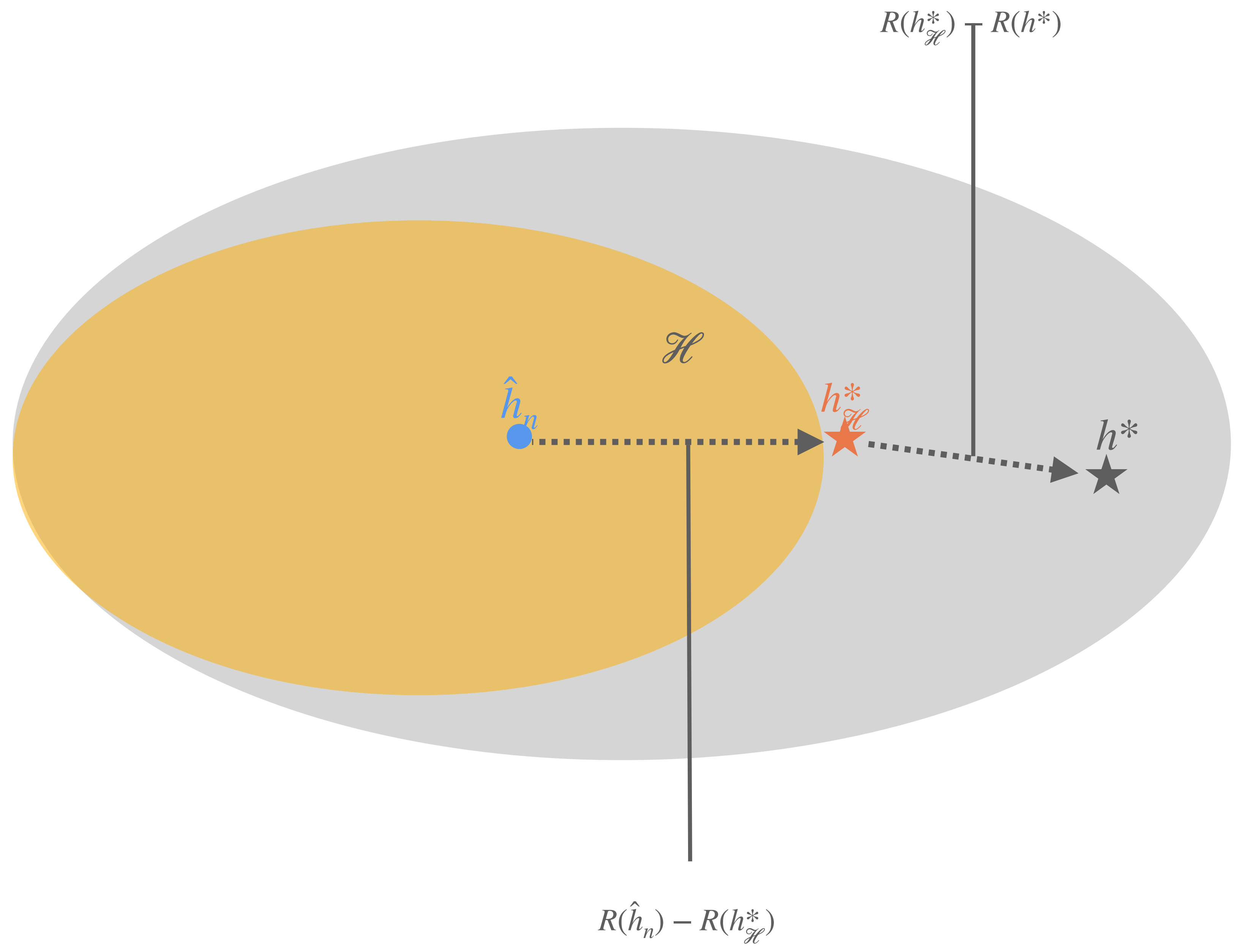
How do we vary the "size" of $\mathcal{H}$ to trade estimation error off with approximation error?

Excess Risk

Intuition: Size of $\mathscr{H}$

$$R(\hat{h}_n) - R(h^*) = \underbrace{R(\hat{h}_n) - R(h^*_{\mathscr{H}})}_{\text{est. error}} + \underbrace{R(h^*_{\mathscr{H}}) - R(h^*)}_{\text{approx. error}}$$


$R(h^*_{\mathscr{H}}) - R(h^*)$
$\mathscr{H}$
$\hat{h}_n$
$h^*_{\mathscr{H}}$
h^*
$R(\hat{h}_n) - R(h^*_{\mathscr{H}})$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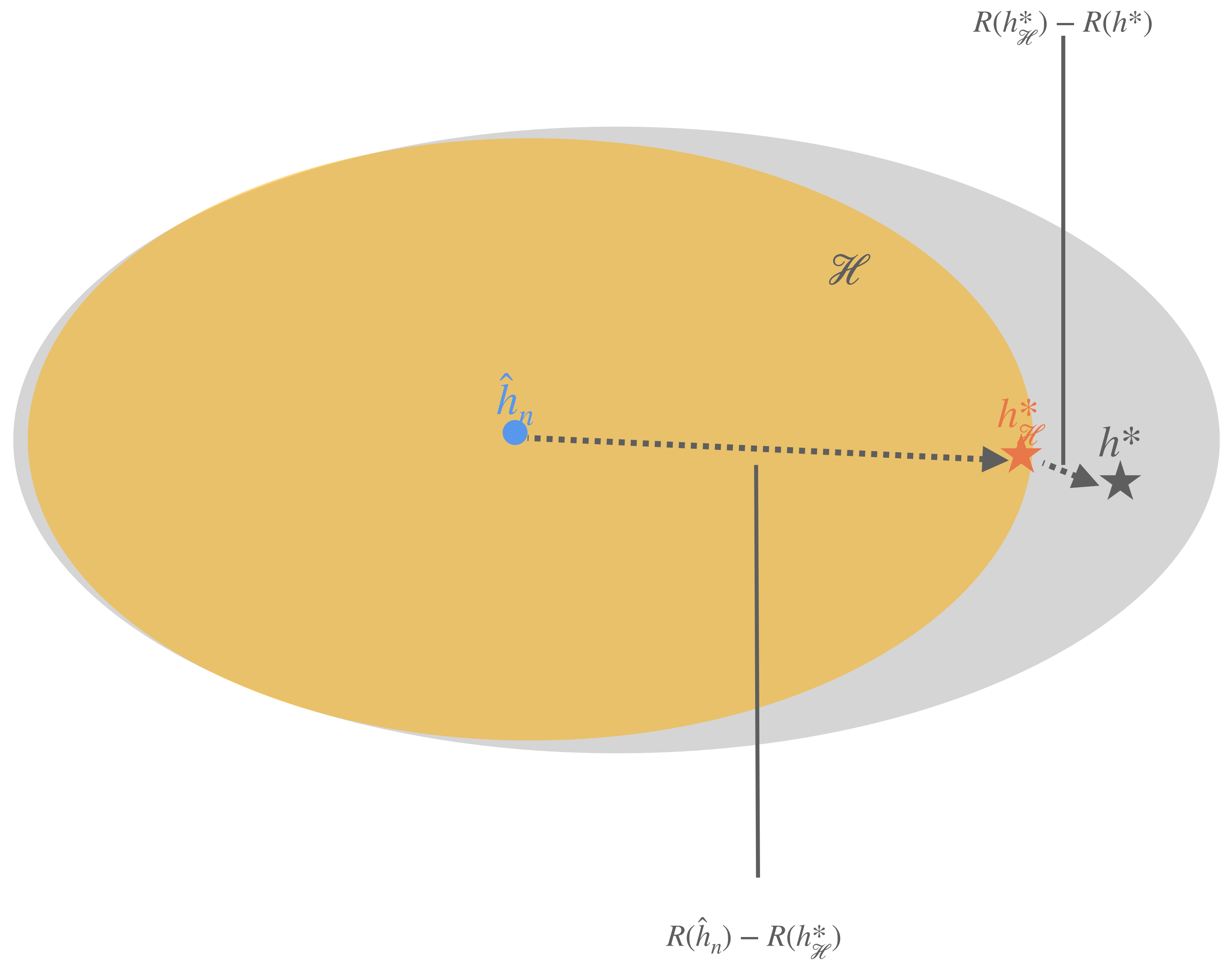
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$\mathscr{H}$
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h^*
$R(\hat{h}_n) - R(h^*_{\mathscr{H}})$

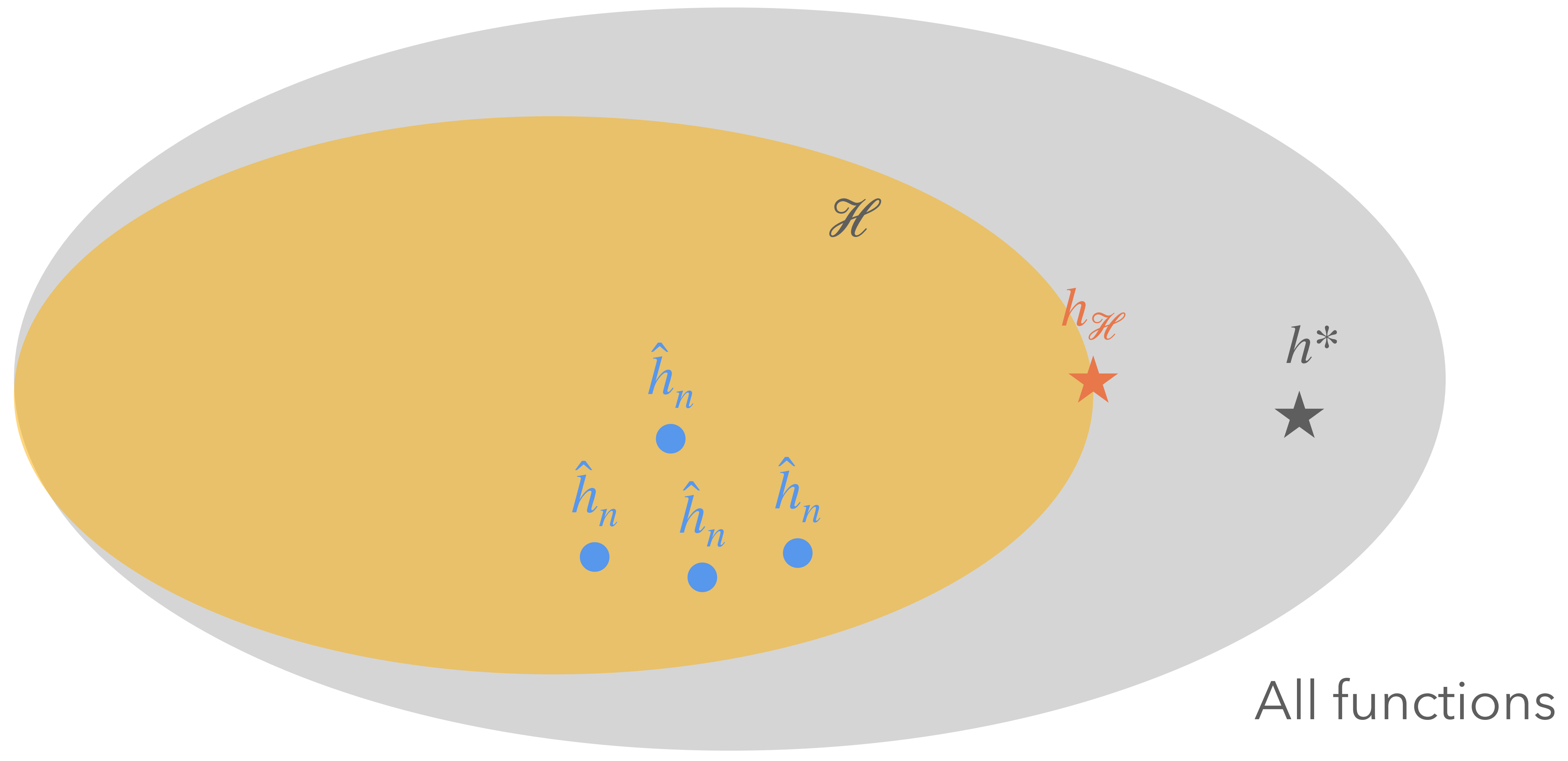
Complexity of $\mathscr{H}$

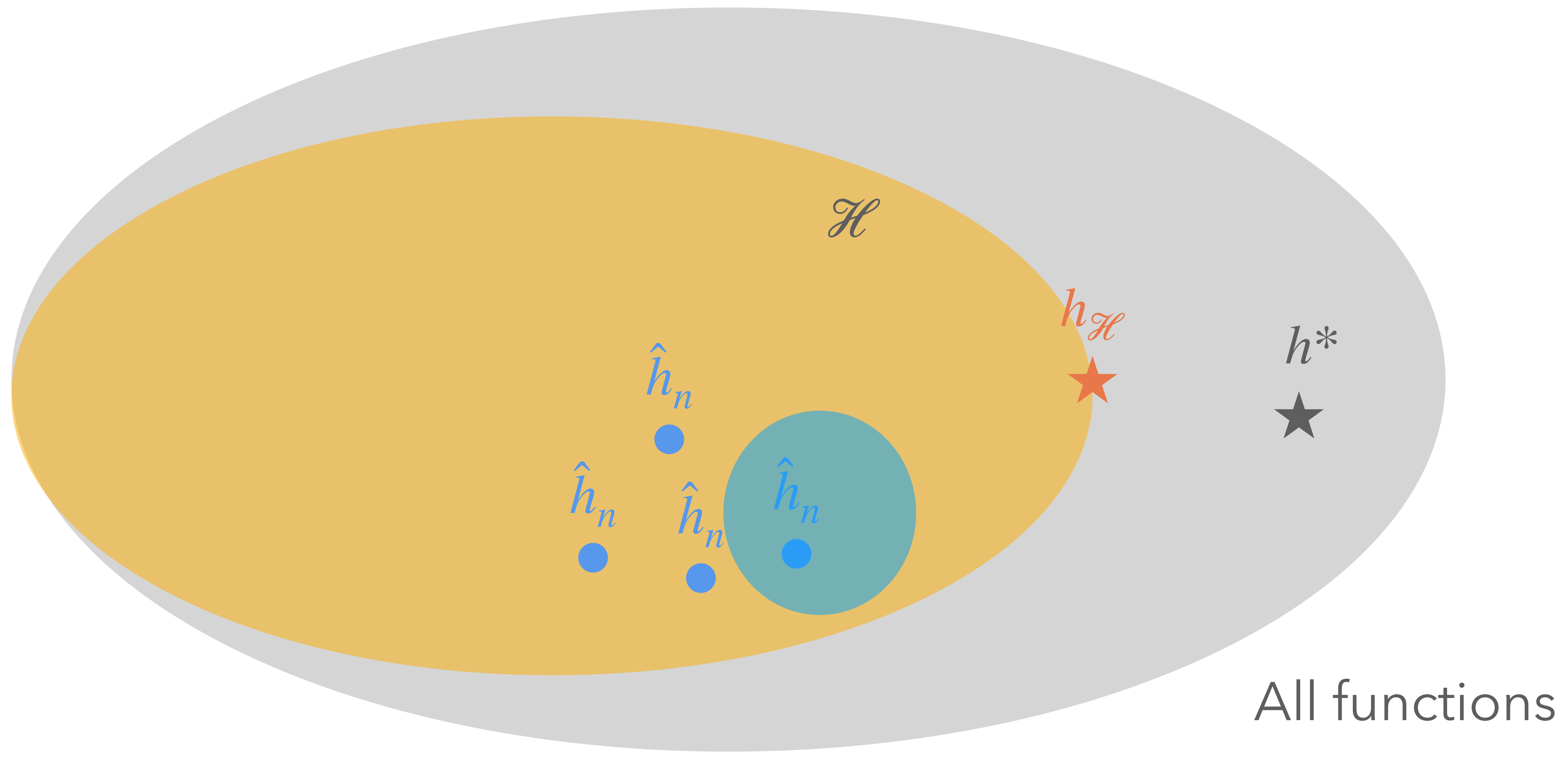
Trade-off

$(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}).$

There can be an infinite number of ERMs!

Regularization: taking a problem with infinitely many solutions and biasing to a smaller ("less complex") subset of solutions.





Controlling Complexity

General Approach

$\mathcal{H}_1 = a_0 + a_1 x$

$\mathcal{H}_2 = a_0 + a_1 x + a_2 x^2$.

1. Learn a sequence of models varying in complexity from the training data.

$$\mathcal{H}_1 \subset \mathcal{H}_2 \subset \ldots \subset \mathcal{H}_n \subset \mathcal{H}$$

Example: Polynomial Functions

$\mathcal{H} = \{$ all polynomial functions$\}$

$\mathcal{H}_d = \{$ all polynomials of degree $\leq d\}$

2. Select one of these models based on a score (e.g. validation error).

Controlling Complexity

Examples for Different Hypotheses

Number of variables/features.

Depth of a decision tree.

Degree of a polynomial.

How about for **linear** decision functions: $x \mapsto \underline{w_1}x_1 + \ldots + \underline{w_d}x_d$?

ℓ_0 complexity: number of non-zero coefficients.

ℓ_1 ("lasso") complexity: $\underline{\underline{\sum |w_i|}}$ for coefficients $w_1, \ldots, w_d$.

ℓ_2 ("ridge") complexity: $\underline{\underline{\sum}} w_i^2$ for coefficients $w_1, \ldots, w_d$.

Linear (Least Squares) Regression

Running Example

Input space: $\mathcal{X} = \mathbb{R}^d$

Hypothesis class is parametrized by $w \in \mathbb{R}^d$

Output space: $\mathcal{Y} = \mathbb{R}$ Action space: $\mathcal{A} = \mathcal{Y} = \mathbb{R}$

Loss Function: $\ell(\hat{y}, y) = (\hat{y} - y)^2$

Hypothesis Class: $\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R} : h(x) = w^\top x, w \in \mathbb{R}^d\}$

Given dataset $D_n := \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$ we want to minimize the empirical risk:

$\hat{R}_n(w) = \dfrac{1}{n}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2$ or $\hat{R}_n(w) = \dfrac{1}{n}\|Xw - y\|^2$ with $X \in \mathbb{R}^{n \times d}$, $y \in \mathbb{R}^n$.

Objective in scalar form

Objective in matrix-vector form

Polynomial Regression

1D Example

$d=1$ $\quad \mathcal{X} = \mathbb{R}$ $\quad \mathcal{Y} = \mathbb{R}$

For a feature $x \in \mathbb{R}$, we can always transform $x \mapsto \phi(x)$ where

$$\phi(x) = \underline{\begin{pmatrix} 1 & x & x^2 & \ldots & x^d \end{pmatrix}}. \in \mathbb{R}^{d+1}$$

Then, fitting a linear model atop transformed features $(\phi(x_1), y_1), \ldots, (\phi(x_n), y_n)$ is a polynomial:

$$w^\top \phi(x) = \underline{w_0} + \underline{w_1}x + \underline{w_2}x^2 + \ldots + \underline{w_d}x^d.$$

Polynomial Regression

1D Example

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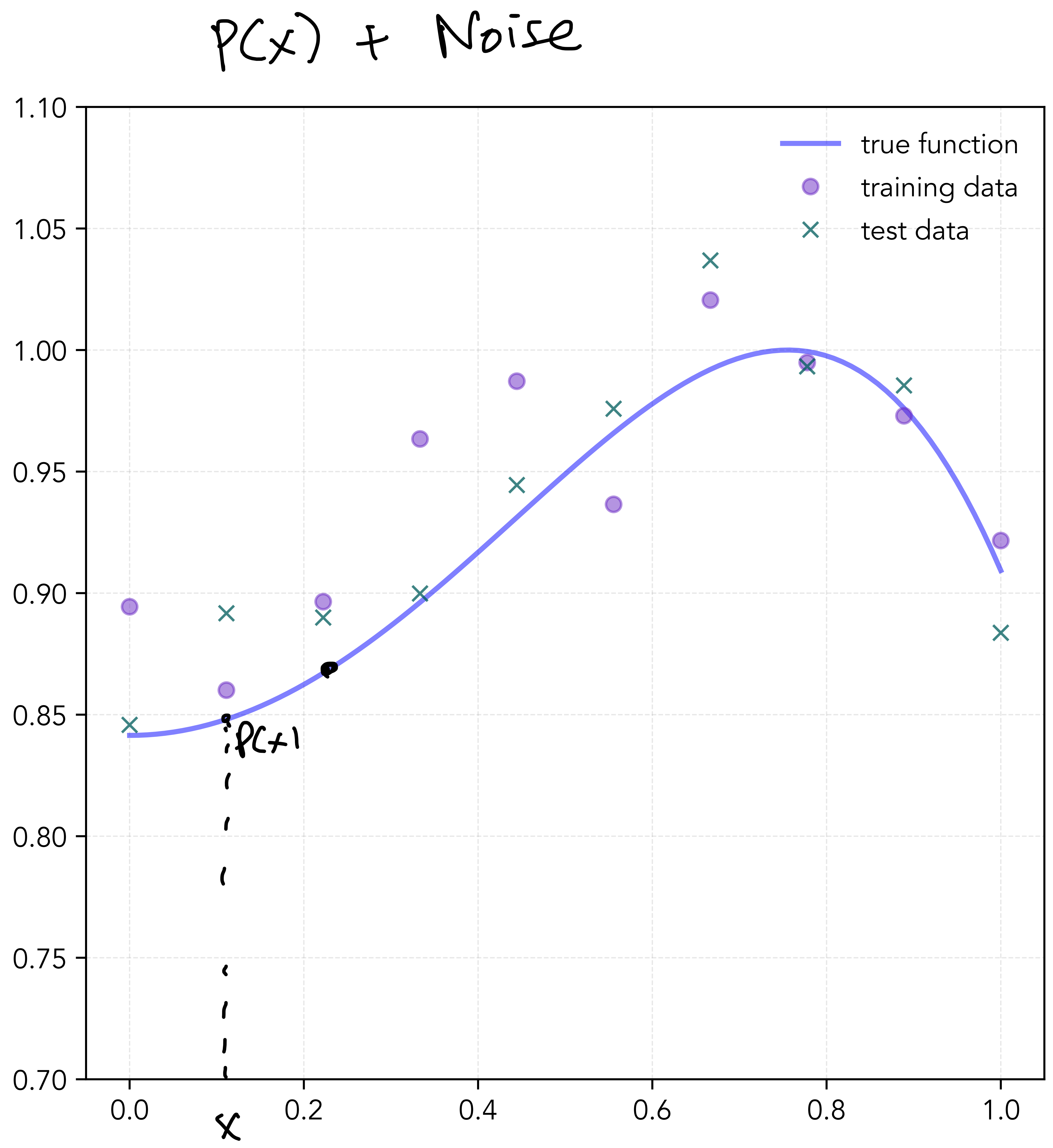


Polynomial Regression

1D Example: Degree 1

For a feature $x \in \mathbb{R}$, we can always transform $x \mapsto \phi(x)$ where:

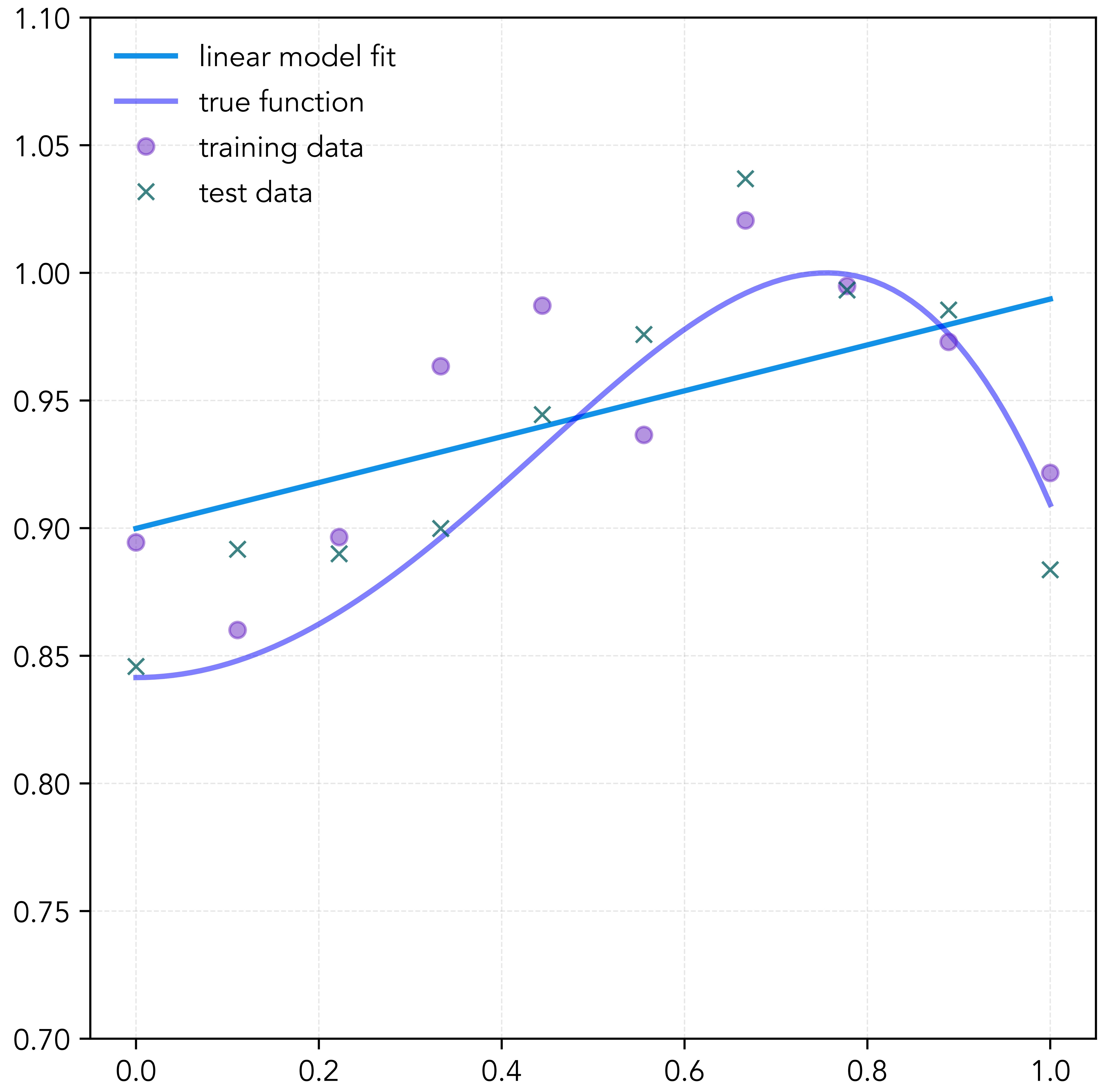
$$\phi(x) = \begin{pmatrix} 1 & x & x^2 & \ldots & x^d \end{pmatrix}.$$

$$w^\top \phi(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_d x^d.$$

Fitting $d = 1$:

$$w^\top \phi(x) = w_0 + w_1 x$$

$$\mathcal{H}_1 = \{ x \mapsto w_0 + w_1 x \}$$



Polynomial Regression

1D Example: Degree 2

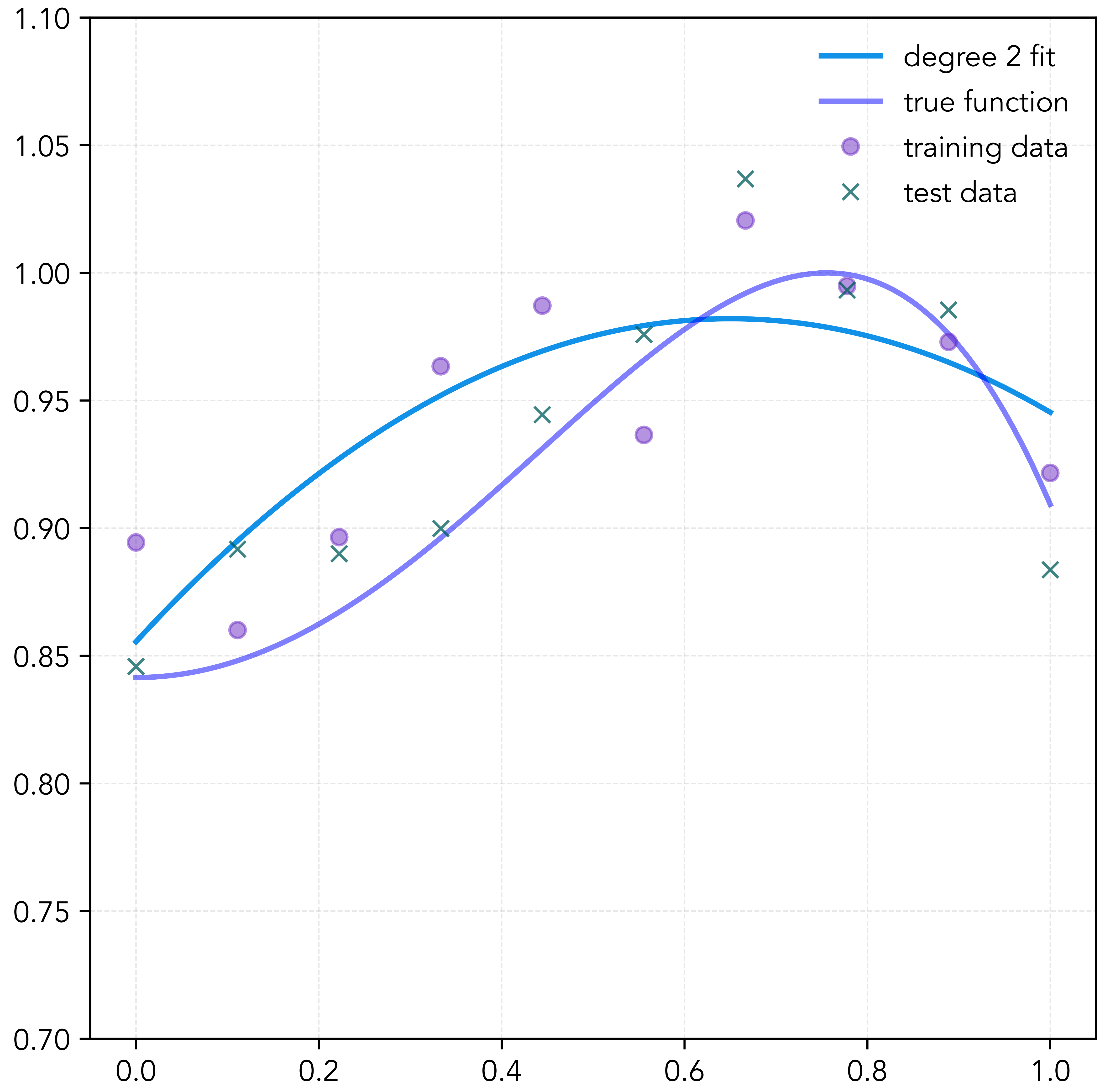
For a feature $x \in \mathbb{R}$, we can always transform $x \mapsto \phi(x)$ where:

$$\phi(x) = \begin{pmatrix} 1 & x & x^2 & \dots & x^d \end{pmatrix}.$$

$$w^\top \phi(x) = w_0 + w_1 x + w_2 x^2 + \dots + w_d x^d.$$

Fitting $d = 2$:

$$w^\top \phi(x) = \underbrace{w_0 + w_1 x}_{\mathcal{H}_1} + w_2 x^2$$



Polynomial Regression

1D Example: Degree 3

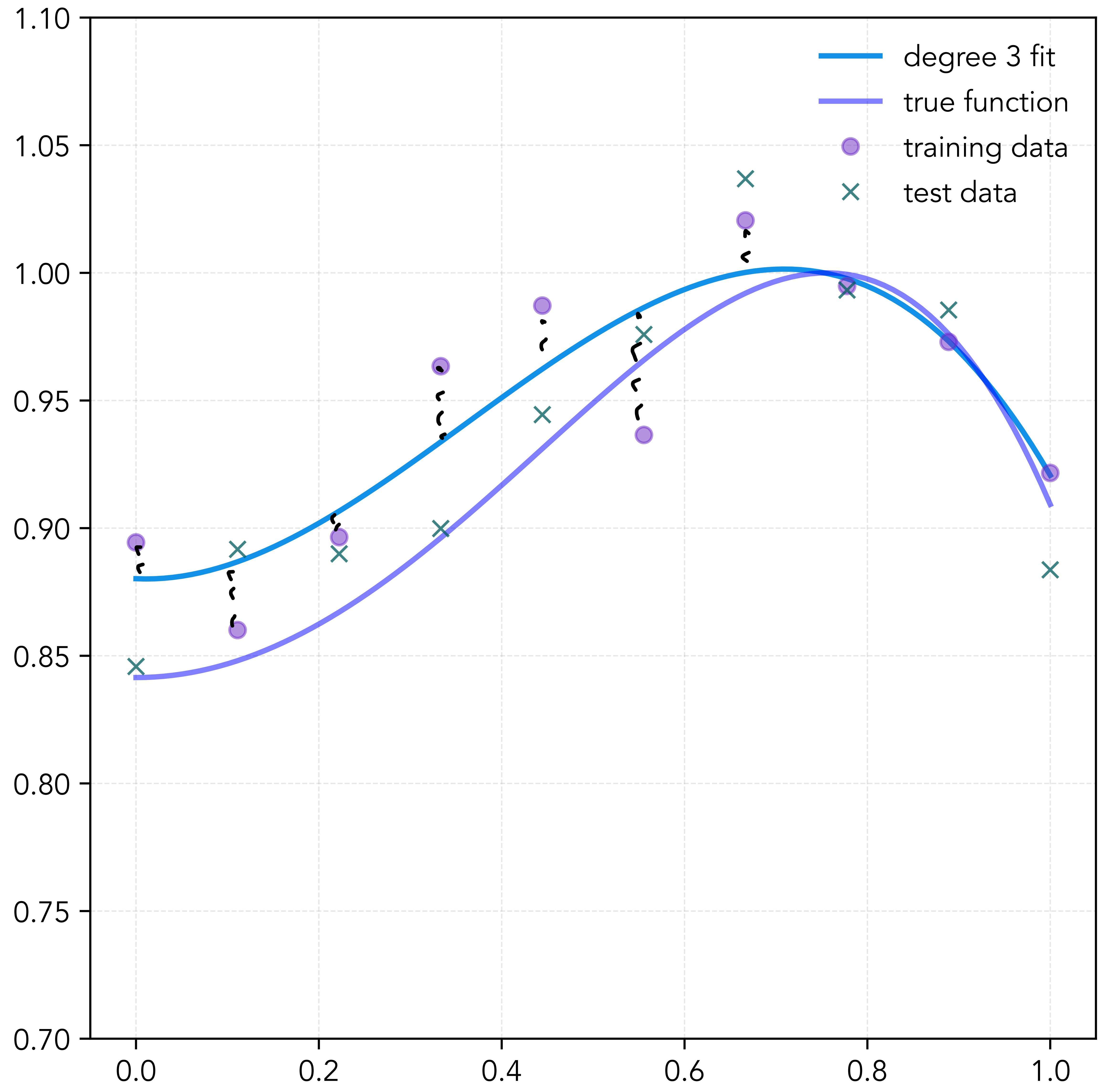
For a feature $x \in \mathbb{R}$, we can always transform $x \mapsto \phi(x)$ where:

$$\phi(x) = \begin{pmatrix} 1 & x & x^2 & \dots & x^d \end{pmatrix}.$$

$$w^\top \phi(x) = w_0 + w_1 x + w_2 x^2 + \dots + w_d x^d.$$

Fitting $d = 3$:

$$w^\top \phi(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



Polynomial Regression

1D Example: Degree 9

For a feature $x \in \mathbb{R}$, we can always transform $x \mapsto \phi(x)$ where:

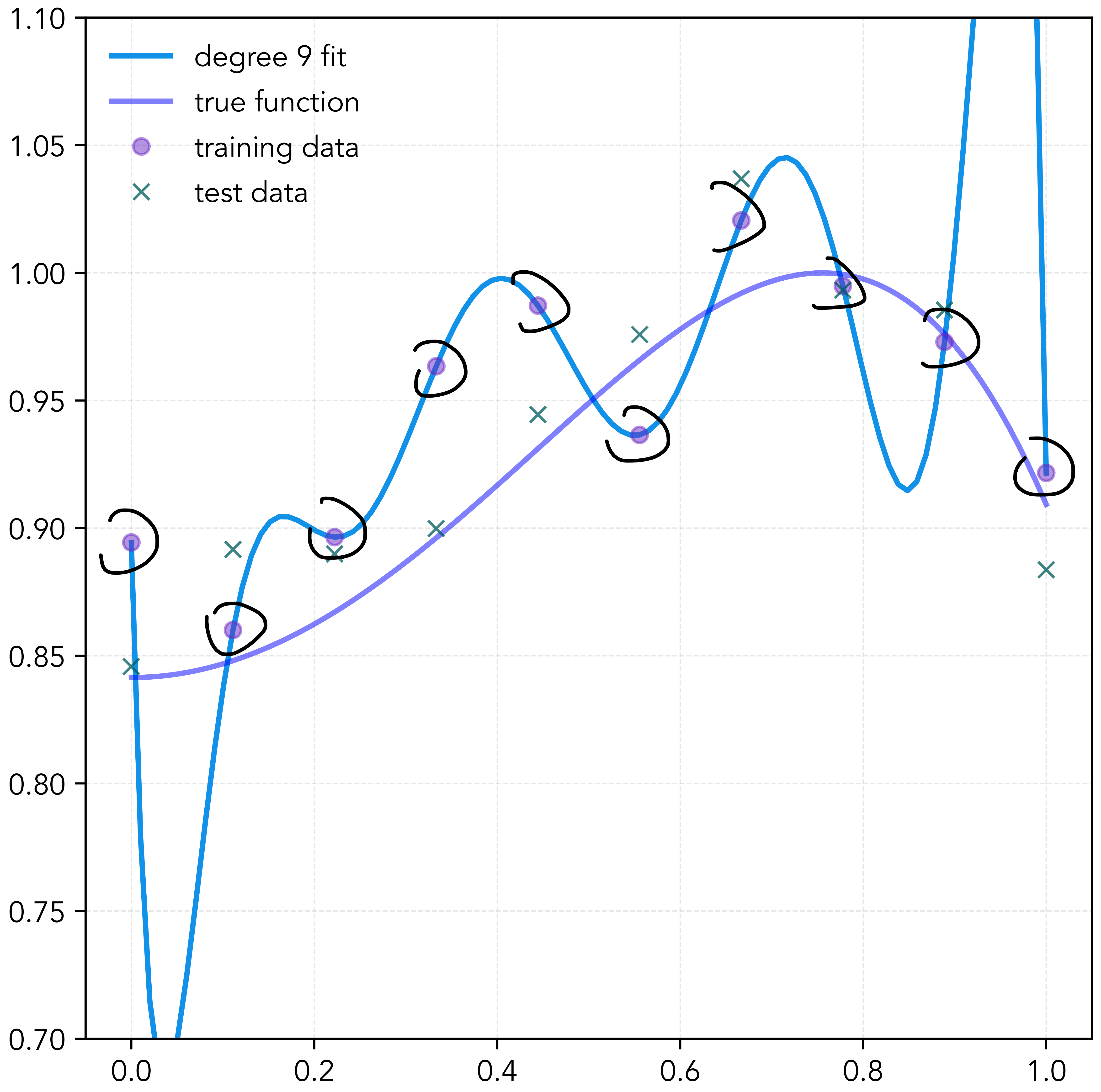
$$\phi(x) = \begin{pmatrix} 1 & x & x^2 & \dots & x^d \end{pmatrix}.$$

$$w^\top \phi(x) = w_0 + w_1 x + w_2 x^2 + \dots + w_d x^d.$$

Fitting $d = 9$:

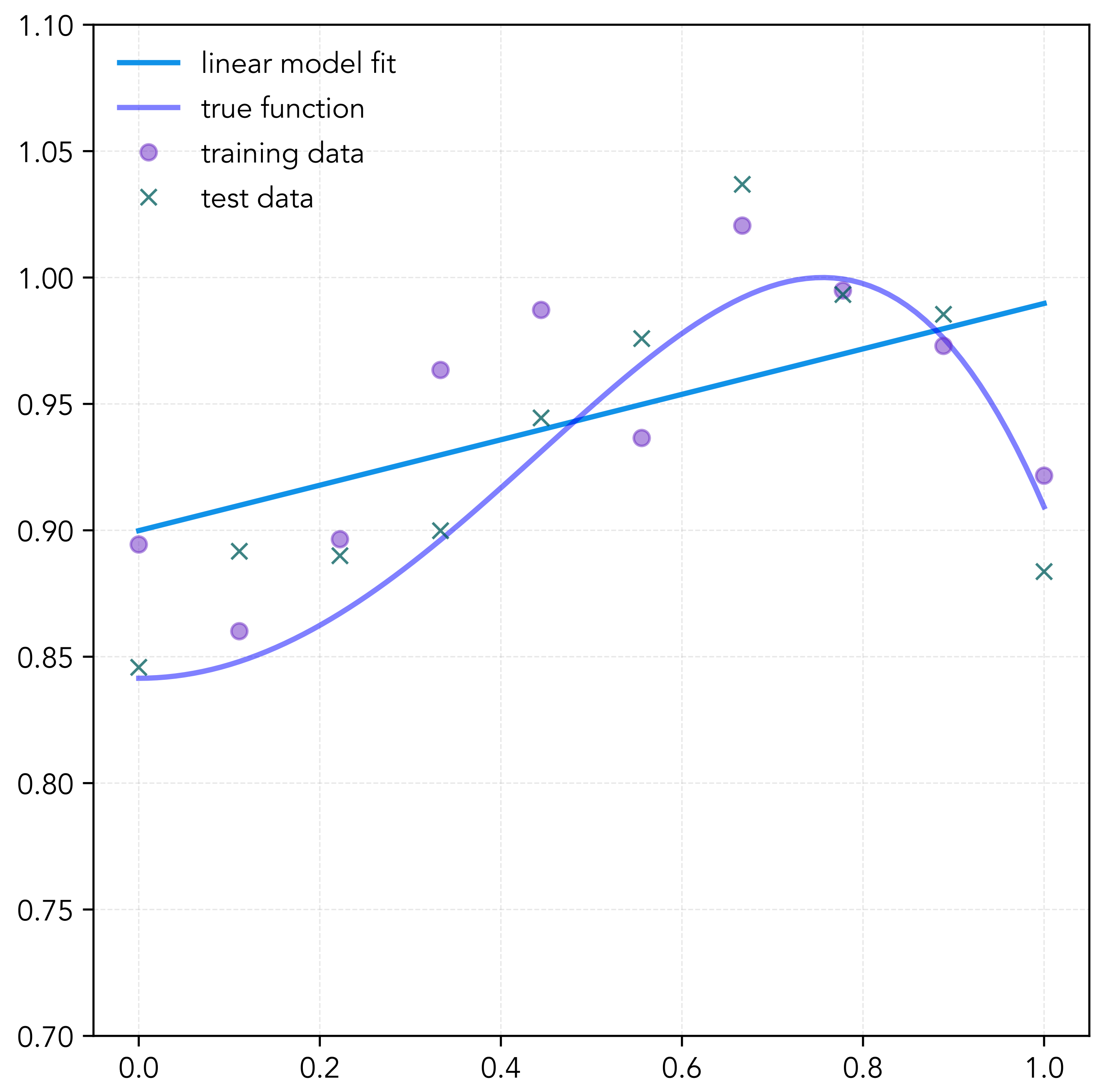
$$\boxed{\underline{w^\top \phi(x) = w_0 + w_1 x + w_2 x^2 + \dots + w_{10} x^9}}$$

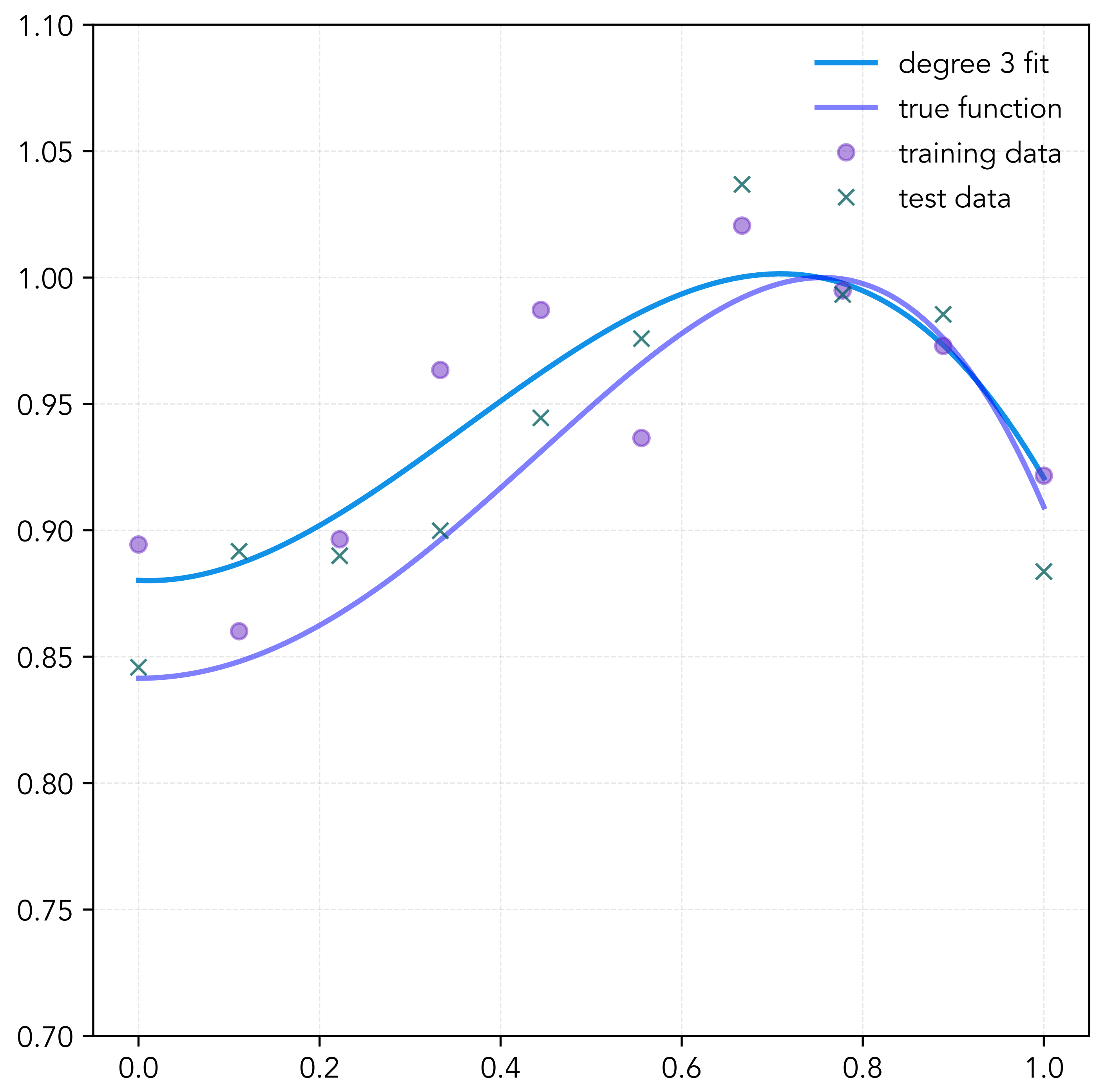
$$\hat{R}_n(\hat{w}) = 0.$$

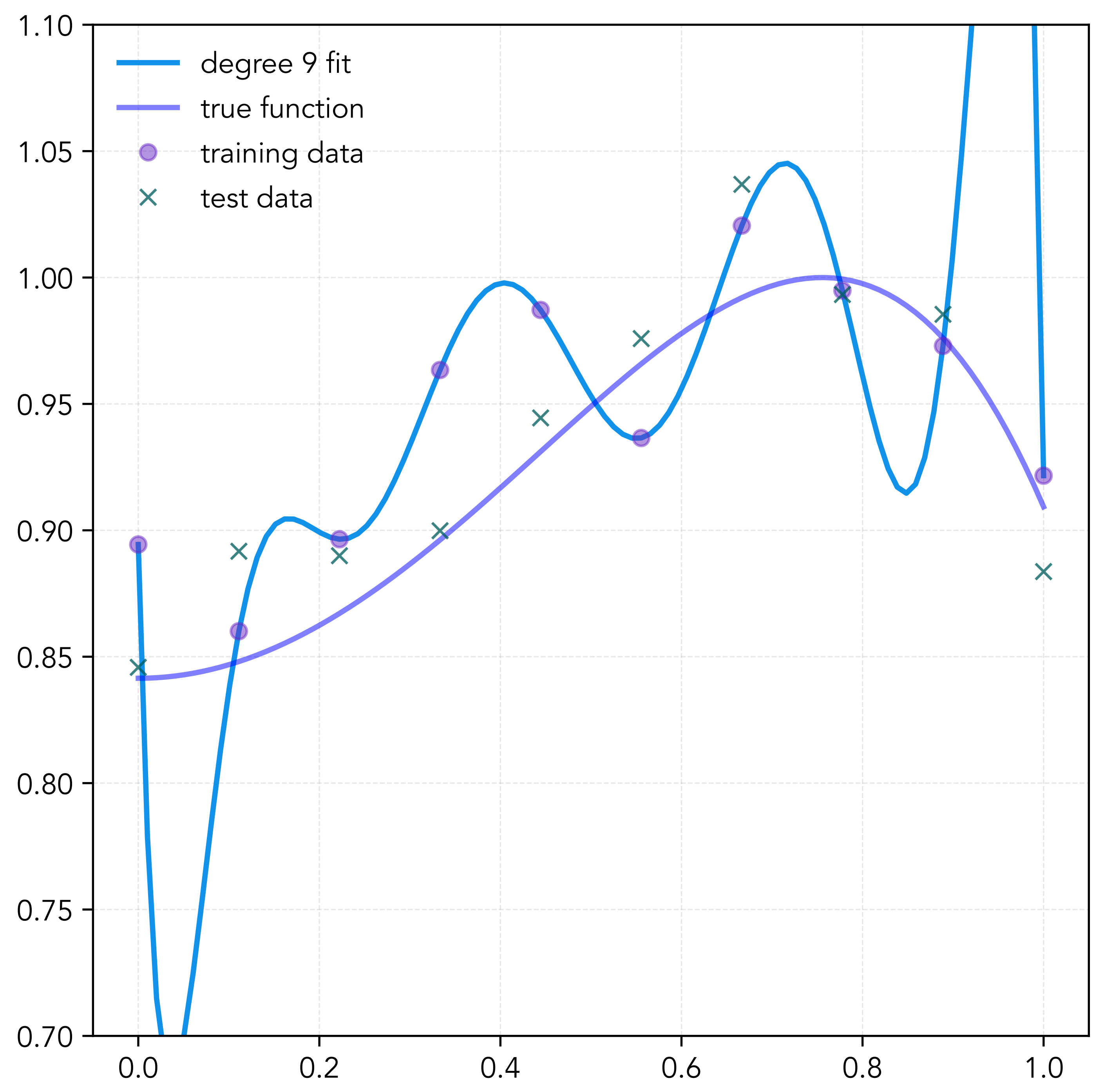


Polynomial Regression

Underfit, Just Right, Overfit







There can be an infinite number of ERMs!

Polynomial Regression

Model Selection

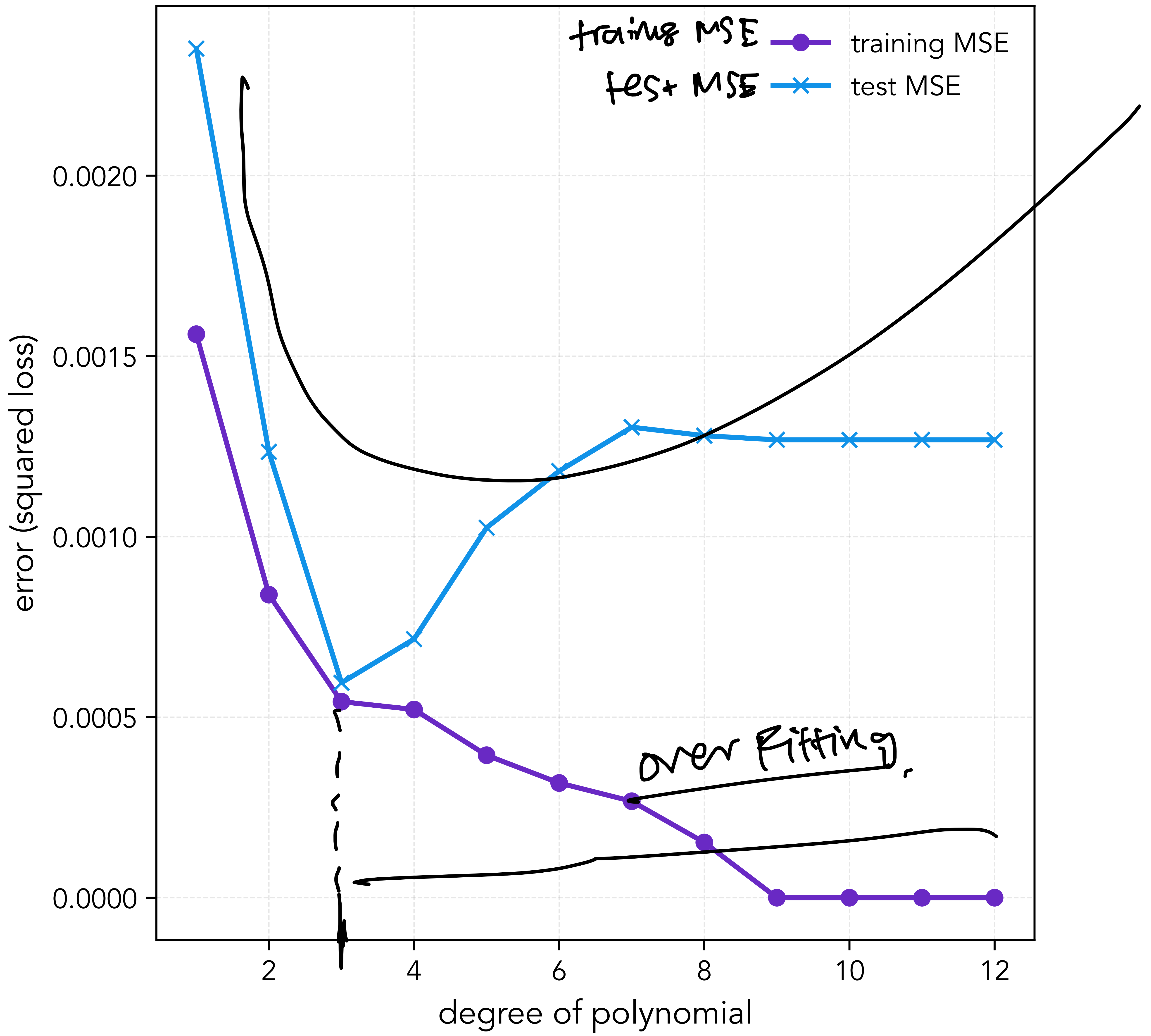
It doesn't take much to drive down empirical risk using polynomials:

$$\hat{R}_n(\hat{h}_n) \approx 0.$$

The more complex our model, the better our empirical risk during training.

Recall:

$$\hat{R}_n(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)})$$



Polynomial Regression

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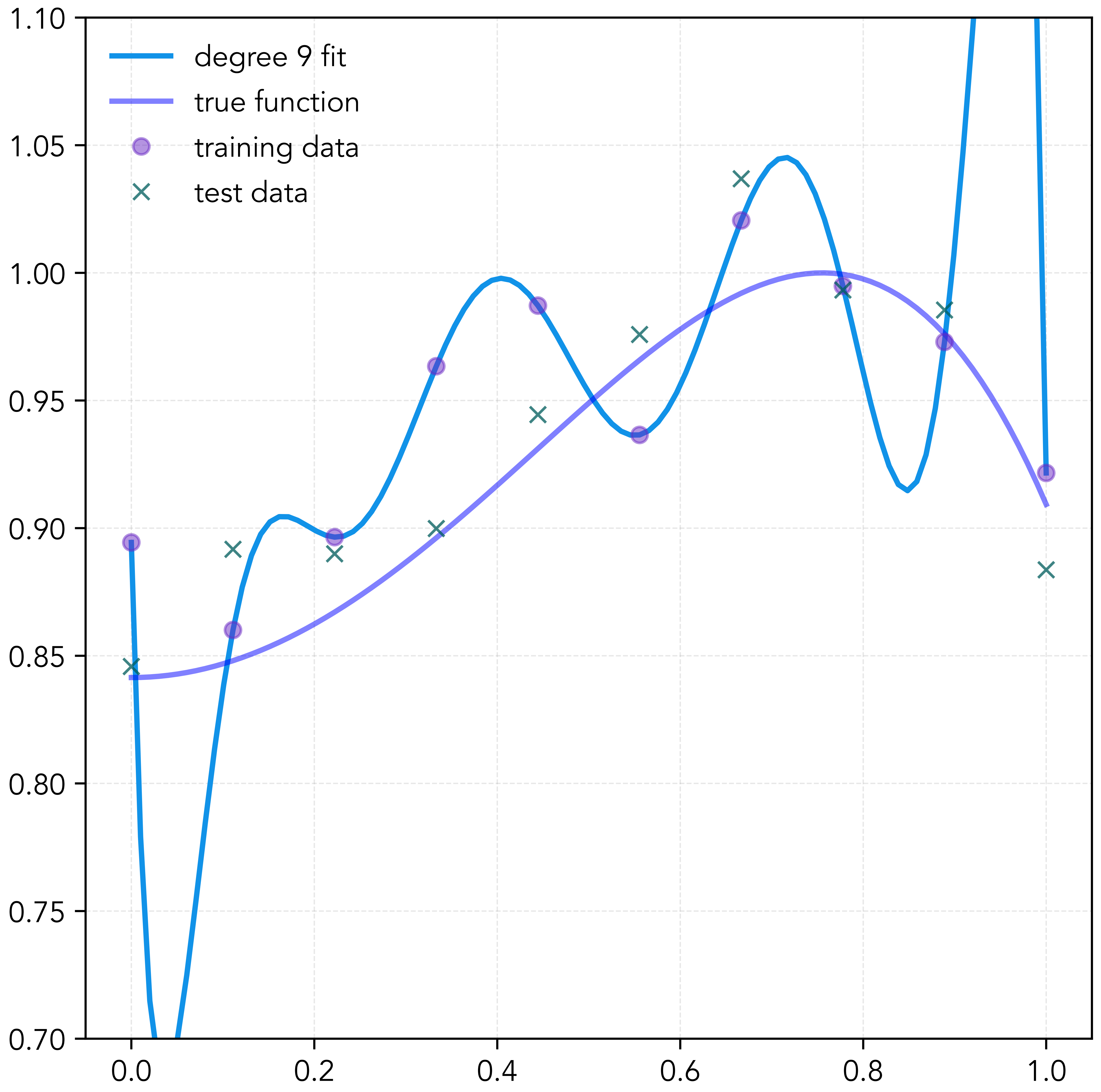
It doesn't take much to drive down empirical risk using polynomials:

$$\hat{R}_n(\hat{h}_n) \approx 0.$$

The more complex our model, the better our empirical risk during training.

But this doesn't mean we'll necessarily do well on *new data*.

We call this overfitting.



Polynomial Regression

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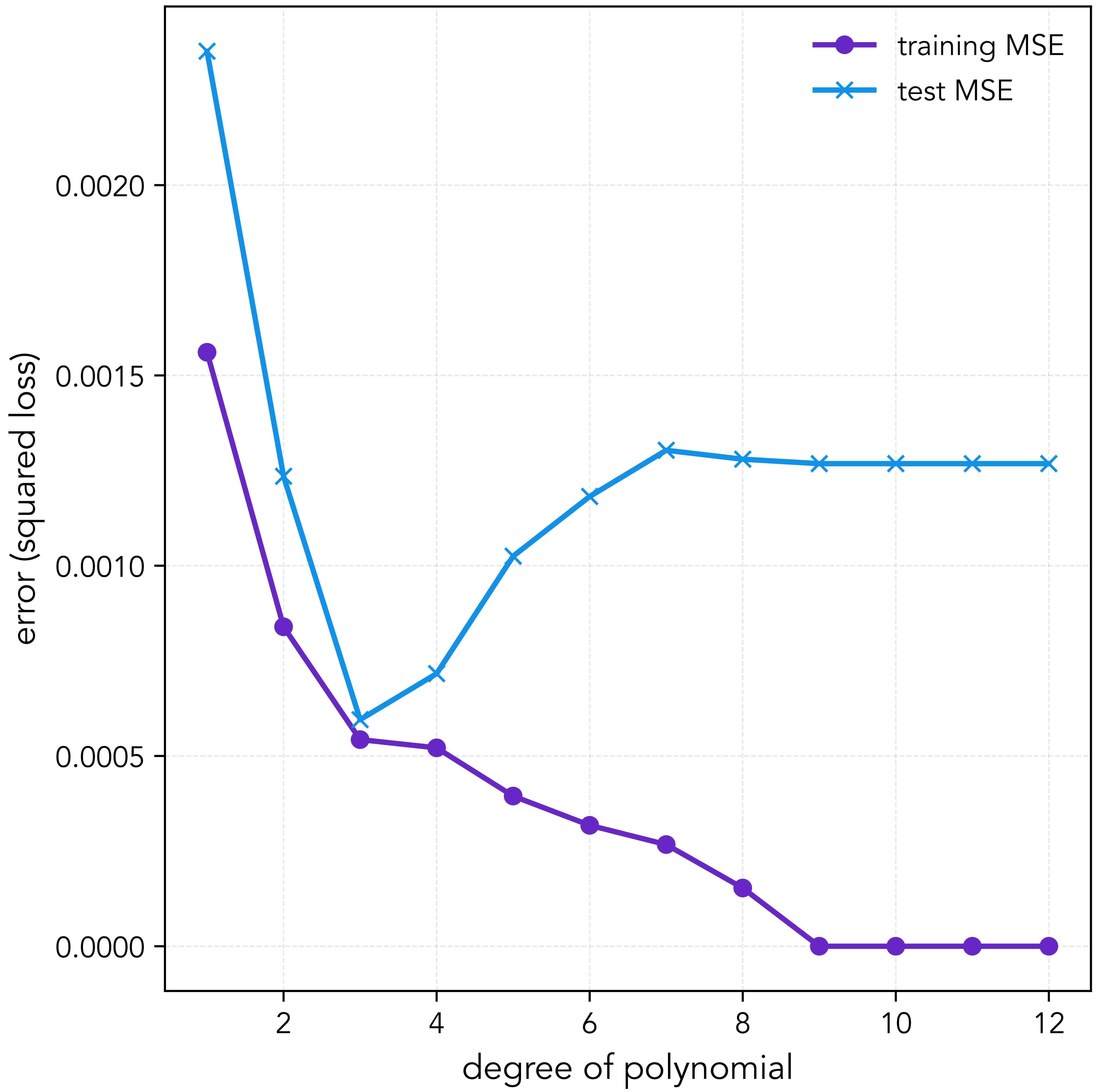


$$\frac{1}{n}\sum_{i=1}^{n} \ell(f^{(1)}(x^{(i)}), y^{(i)}) \approx \mathbb{E}[\ell(f^{(1)}(x), y)$$

Polynomial Regression

Model Selection

In practice, we can directly test a model on "new data" (unseen in training).

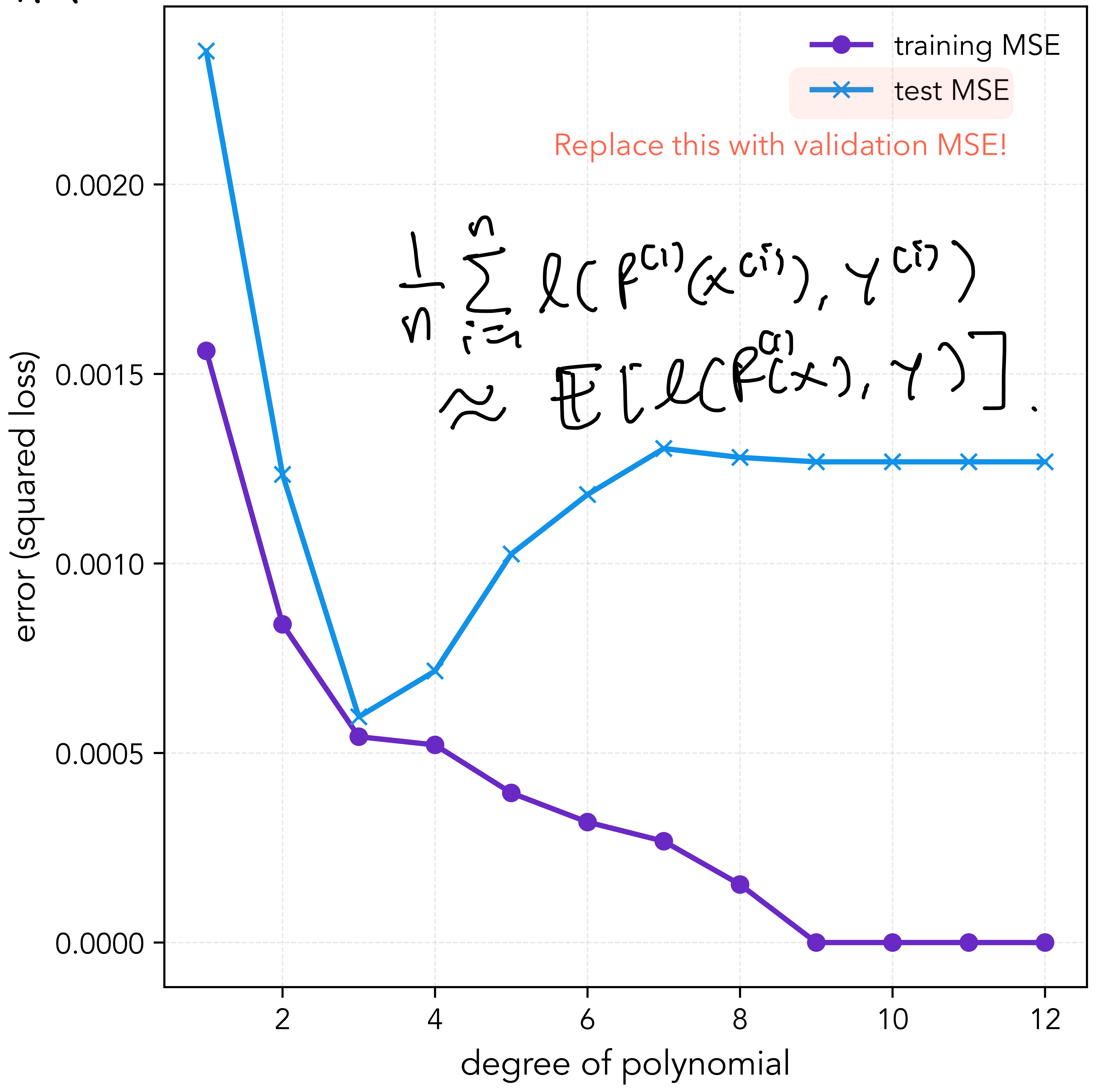
Model selection on a **validation set:**

1. Split training set D_n into **train set** D_n^1 and **validation set** D_n^2.

2. Train k models $f^{(1)}, \ldots, f^{(k)}$ of varying complexity using D_n^1.

3. Evaluate each of $f^{(1)}, \ldots, f^{(k)}$ on D_n^2.

4. Pick model with lowest validation loss.



Replace this with validation MSE!

$$\frac{1}{n}\sum_{i=1}^{n} \ell(f^{(1)}(x^{(i)}), y^{(i)}) \approx \mathbb{E}[\ell(f^{(1)}(x), y)].$$

Polynomial Regression

Model Selection

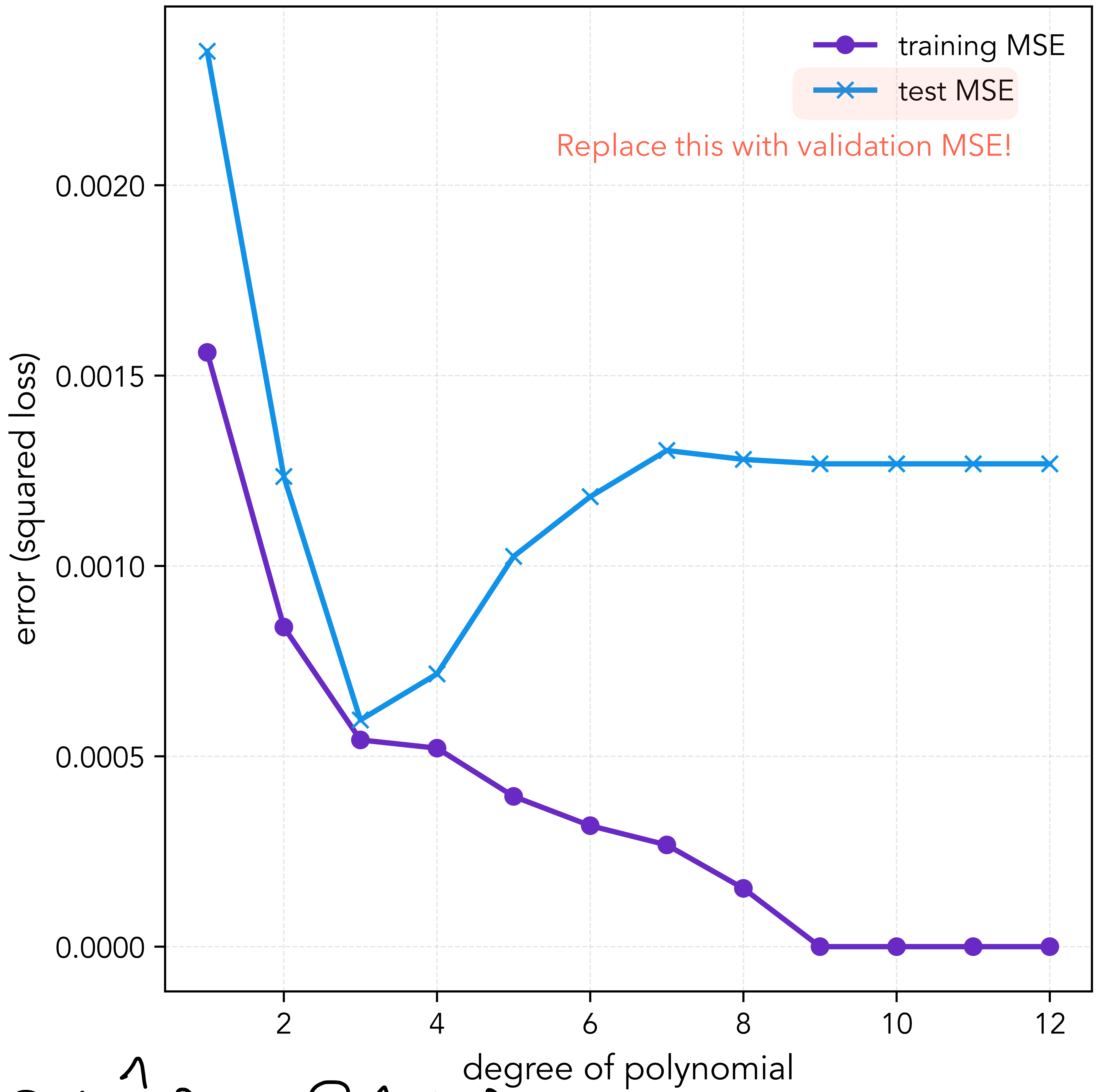
Split training set D_n into **train set** D_n^1 and **validation set** D_n^2

$$D_n^1 = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$$

$$D_n^2 = \{(\tilde{x}^{(1)}, \tilde{y}^{(1)}), \ldots, (\tilde{x}^{(m)}, \tilde{y}^{(m)})\}$$

As long as $\hat{h}_n$ is chosen without ~~looking~~ training at D_n^2, we have an estimate of **true risk.**

$$\frac{1}{n}\sum_{j=1}^{n} \ell(h(\tilde{x}^{(j)}), \tilde{y}^{(j)}) \approx \underline{\mathbb{E}[\ell(h(x), y)] = R(h)}$$



$R(\hat{h}_n) - R(h^*_{\mathcal{H}})$

Outline

Controlling Complexity

Feature Selection in Linear Regression $x \mapsto \quad w_0 + \cancel{w_1} x_1 + \dots + \cancel{w_d} x_d$

ℓ_0 complexity: number of non-zero coefficients.

$$\mathscr{H}_1 \subset \mathscr{H}_2 \subset \dots \subset \mathscr{H}_n \subset \mathscr{H}$$

Example: Linear Functions

$\mathscr{H}$ = { linear functions using all features}

$\mathscr{H}_d$ = { linear functions using fewer than d features }

$(w_0, 0, 0 \dots, 0)$
$(w_0, w_1, 0, \dots, 0)$
$(w_0, 0, w_2, \dots, 0)$

Best subset selection: Choose subset of features that is best according to score (e.g. validation error). Example with two features: train models using $\{\}$, $\{x_1\}$, $\{x_2\}$ and $\{x_1, x_2\}$.

This is not an efficient search algorithm! 2^d subsets if total of d features.

Controlling Complexity

Feature Selection in Linear Regression

Best subset selection: Choose subset of features that is best according to score (e.g. validation error). Example with two features: train models using $\{\}$, $\{x_1\}$, $\{x_2\}$ and $\{x_1, x_2\}$.

Objective that balances number of feature with performance:

$$\text{score}(S) = \text{train\_loss}(S) + \lambda \left| S \right|$$

λ balances the training loss and the number of features used.

Adding an extra feature must be justified with λ improvement in training loss.

Larger λ: complex models penalized more heavily.

Complexity Penalty

Constrained ERM (Ivanov Regularization)

Goal: Balance the complexity of the hypothesis class $\mathscr{H}$ and its training loss.

For complexity measure $\underline{\Omega : \mathscr{H} \to [0,\infty)}$ and fixed $r \geq 0$, the constrained ERM problem is:

$$\boxed{\min_{h \in \mathscr{H}}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)})$$

$$\boxed{\text{s.t.} \quad \Omega(\cancel{f}\, h) \leq \boxed{r}}$$

Find r using performance on validation data.

Each r corresponds to different hypothesis classes. Could also write: $\min_{\underline{h \in \mathscr{H}_r}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)})$

Complexity Penalty

Penalized ERM (Tikhonov Regularization)

Goal: Balance the complexity of the hypothesis class $\mathscr{H}$ and its training loss.

For complexity measure $\Omega : \underline{\mathscr{H}} \to \underline{[0,\infty)}$ and fixed $r \geq 0$, the penalized ERM problem is:

$$\boxed{\min_{h\in\mathscr{H}}} \frac{1}{n}\sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}) + \underline{\lambda\Omega(h)}$$

Big $\Rightarrow$ Discourage from choosing h.

Price you're paying for h.

Find λ using performance on validation data.

Penalized vs. Constrained Optimization

In General

Let $L : \mathcal{H} \to \mathbb{R}$ be *any* performance measure of h (e.g. empirical risk).

For many L and Ω, constrained and penalized regularization are "equivalent":

For any $r > 0$, $h_r^* \in \underset{h \in \mathcal{H}}{\arg\min}\ L(h)$ s.t. $\Omega(h) \leq r$ is in $\underset{h \in \mathcal{H}}{\arg\min}\ L(h) + \lambda\Omega(h)$ for some $\lambda > 0$.

For any $\lambda > 0$, $h_\lambda^* \in \underset{h \in \mathcal{H}}{\arg\min}\ L(h) + \lambda\Omega(h)$ is in $\underset{h \in \mathcal{H}}{\arg\min}\ L(h)$ s.t. $\Omega(h) \leq r$ for some $r > 0$.

In practice, both approaches are effective.

Penalized regularization convenient because it's an *unconstrained* optimization problem.

Can often run gradient Descent.

Complexity Penalty

Penalized ERM (Tikhonov Regularization)

Goal: Balance the complexity of the hypothesis class $\mathscr{H}$ and training loss.

For complexity measure $\Omega : \mathscr{H} \to [0,\infty)$ and fixed $r \geq 0$, the penalized ERM problem is:

$$\min_{h \in \mathscr{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}) + \lambda \Omega(h)$$

Setting $\Omega(\cdot)$ as "number of features" is not differentiable and hard to optimize.

What other measures of complexity can we use?

Outline

"Soft" Selection

Linear Regression

Input space: $\mathcal{X} = \mathbb{R}^d$

Output space: $\mathcal{Y} = \mathbb{R}$

$$\underline{w_0} x_1 + \underline{w_1} x_1 + \dots + \underline{w_d} x_d$$

Loss Function: $\ell(\hat{y}, y) = (\hat{y} - y)^2$

Hypothesis Class: $\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R} : h(x) = w^\top x, w \in \mathbb{R}^d\}$

Imagine having a weight for each feature dimension.

In linear regression, model weights multiply each feature dimension.

If w_i is close to zero, then it means we aren't using feature i.

Linear Regression

Running Example

Input space: $\mathcal{X} = \mathbb{R}^d$; Output space: $\mathcal{Y} = \mathbb{R}$; Loss Function: $\ell(\hat{y}, y) = (\hat{y} - y)^2$

Hypothesis Class: $\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R} : h(x) = w^\top x, w \in \mathbb{R}^d\}$

Given dataset $D_n := \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$ we want to minimize the empirical risk:

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

This often overfits, especially when $d \gg n$! $\rightarrow$

When $d >> n$:

You have infinitely many solutions.

(e.g. in NLP one can have 1M features for 10K documents)

Ridge Regression

$\Omega(w) = \|w\|^2$

Constrained and Penalized ERM

The (penalized form) ridge regression solution with regularization parameter $\lambda \geq 0$ is

$$\hat{w} \in \arg\min_{w \in \mathbb{R}^d} \left(\underbrace{\frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2}_{} + \underline{\underline{\lambda \|w\|_2^2}} \right)$$

Penalize by $\|w\|^2$

where $\|w\|_2^2 = w_1^2 + \ldots + w_d^2$ is the squared ℓ_2-norm.

The (constrained form) ridge regression solution with regularization parameter $r^2 \geq 0$ is

$$\hat{w} \in \arg\min_{\underline{\underline{\|w\|_2^2 \leq r^2}}} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

Ridge Regression

Penalized ERM

The (penalized form) ridge regression solution with regularization parameter $\lambda \geq 0$ is

$$\hat{w} \in \arg\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2 + \lambda \|w\|_2^2$$

where $\|w\|^2 = w_1^2 + \ldots + w_d^2$ is the squared ℓ_2-norm.

Equivalent to linear least squares regression with $\lambda = 0$.

ℓ_2 regularization can be used for other models too (e.g. neural networks).

Sensitivity to Inputs

Effect of Regularization

$$\boxed{|f(x+h) - f(x)| \leq L \, \|h\|}$$

$$\updownarrow$$

$\underline{h(x) = \hat{w}^\top x}$ is Lipschitz continuous with Lipschitz constant $L = \|\hat{w}\|_2$: when moving from $\underline{\underline{x \text{ to } x + \Delta}}$, h changes no more than $L\|\Delta\|$, because:

$$\underline{\left| h(x+\Delta) - h(x) \right|} = \left| \hat{w}^\top (x+\Delta) - \hat{w}^\top x \right| = | \cancel{w^T x} + w^T \Delta - \cancel{w^T x} |$$
$$= \left| \hat{w}^\top \Delta \right| \leq \|\hat{w}\| \|\Delta\|$$

Cauchy-Schwarz Inequality

So ℓ_2 regularization controls the maximum rate of change of h. Same for ℓ_1 Norm.

Other norms also provide a bound on L due to equivalence of norms:

For any p, $\exists C > 0$ such that $\|\hat{w}\|_2 \leq C\|\hat{w}\|_p$.

Linear vs. Ridge Regression

Analytical Comparison

$\longleftarrow$

Linear objective: $\frac{1}{2}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2$

in matrix-vector form: $\frac{1}{2}\|Xw - y\|_2^2$

Gradient: $\nabla L(w) = X^\top(Xw - y)$

Closed-form solution:

$\underline{\underline{n \geq d}}$ $\underline{\hat{w} = (X^\top X)^{-1}X^\top y}$ if X is full rank.

Ridge objective: $\left(\frac{1}{2}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2 + \frac{\lambda}{2}\|w\|_2^2\right)$

in matrix-vector form: $\frac{1}{2}\|Xw - y\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$

Gradient: $\nabla L(w) = X^\top(Xw - y) + \lambda w$

Closed-form solution:

$\underline{d > n}$ $\hat{w} = (X^\top X + \lambda I)^{-1}X^\top y$

($X^\top X + \lambda I$ is always invertible)

Ridge Regression

Constrained and Penalized ERM

The (penalized form) ridge regression solution with regularization parameter $\lambda \geq 0$ is

$$\hat{w} \in \arg\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2 + \lambda \|w\|_2^2$$

where $\|w\|^2 = w_1^2 + \ldots + w_d^2$ is the squared ℓ_2-norm.

The (constrained form) ridge regression solution with regularization parameter $r^2 \geq 0$ is

$$\hat{w} \in \arg\min_{\|w\|_2^2 \leq r^2} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

Linear vs. Ridge

Regularization Path Comparison

$\boxed{\|w\|_2^2 \le r}$

$\boxed{w = (w_1, w_2, w_3, w_4, w_5)}$

No Regularization

Regularized.

$$\boxed{\hat{w}_r \in \underset{\|w\|_2^2 \le r^2}{\arg\min} \frac{1}{n}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2}$$

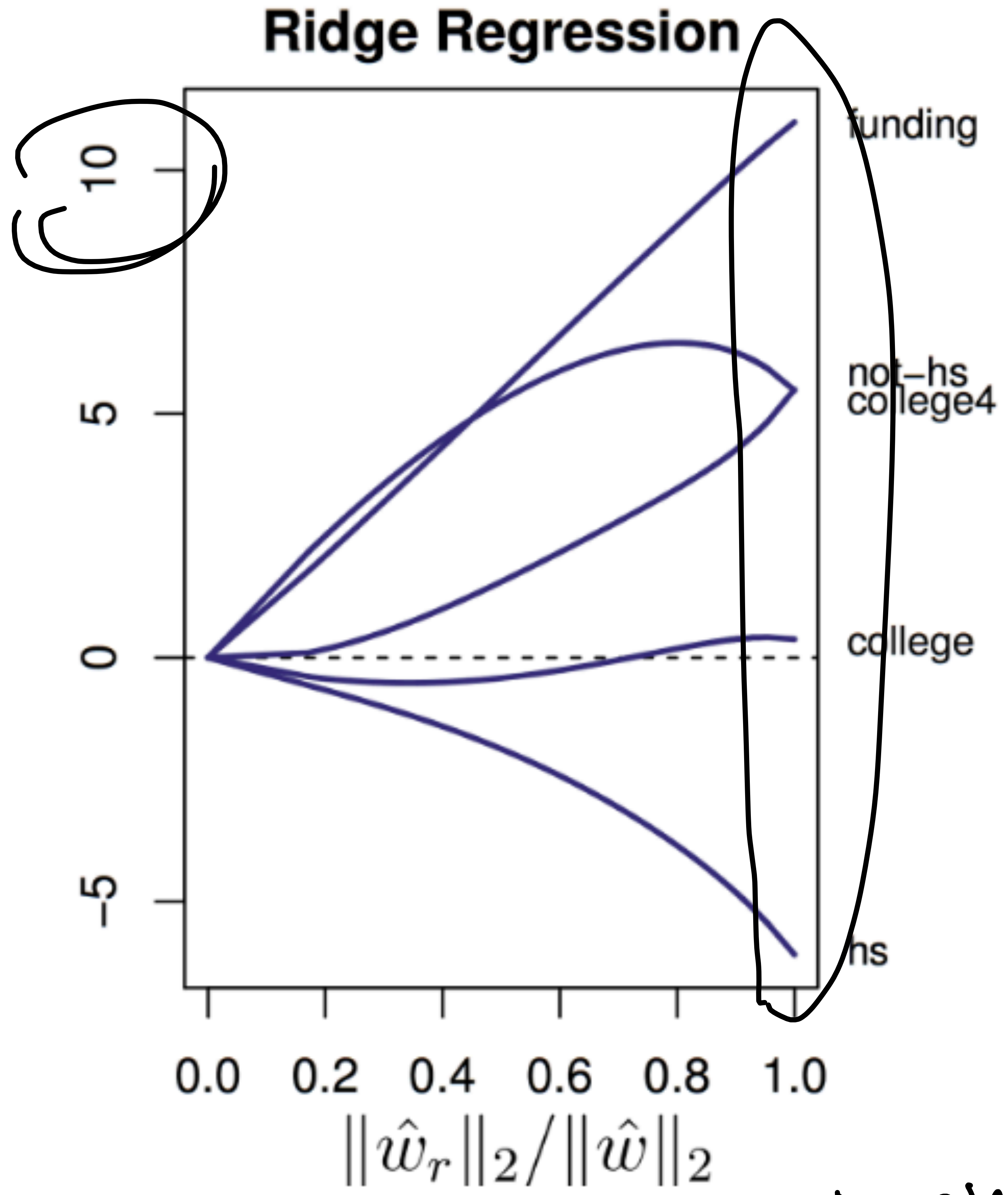
unreg

$$\boxed{\hat{w} \in \underset{w\in\mathbb{R}^d}{\arg\min} \frac{1}{n}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2}$$

For $r = 0$, $\|\hat{w}_r\|_2/\|\hat{w}\|_2 = 0$.

For $\underline{r = \infty}$, $\|\hat{w}_r\|_2/\|\hat{w}\|_2 = 1$.

Regularized. unregularized.



$\longrightarrow$ choosing larger r.

Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

Outline

Lasso Regression

Constrained and Penalized ERM

The (penalized form) lasso regression solution with regularization parameter $\lambda \geq 0$ is

$$\boxed{\hat{w} \in \arg\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2 + \underline{\underline{\lambda \|w\|_1}}}$$

where $\boxed{\|w\|_1 = |w_1| + \ldots + |w_d|}$ is the ℓ_1-norm.

The (constrained form) lasso regression solution with regularization parameter $r \geq 0$ is

$$\hat{w} \in \arg\min_{\|w\|_1 \leq r} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

Linear vs. Ridge

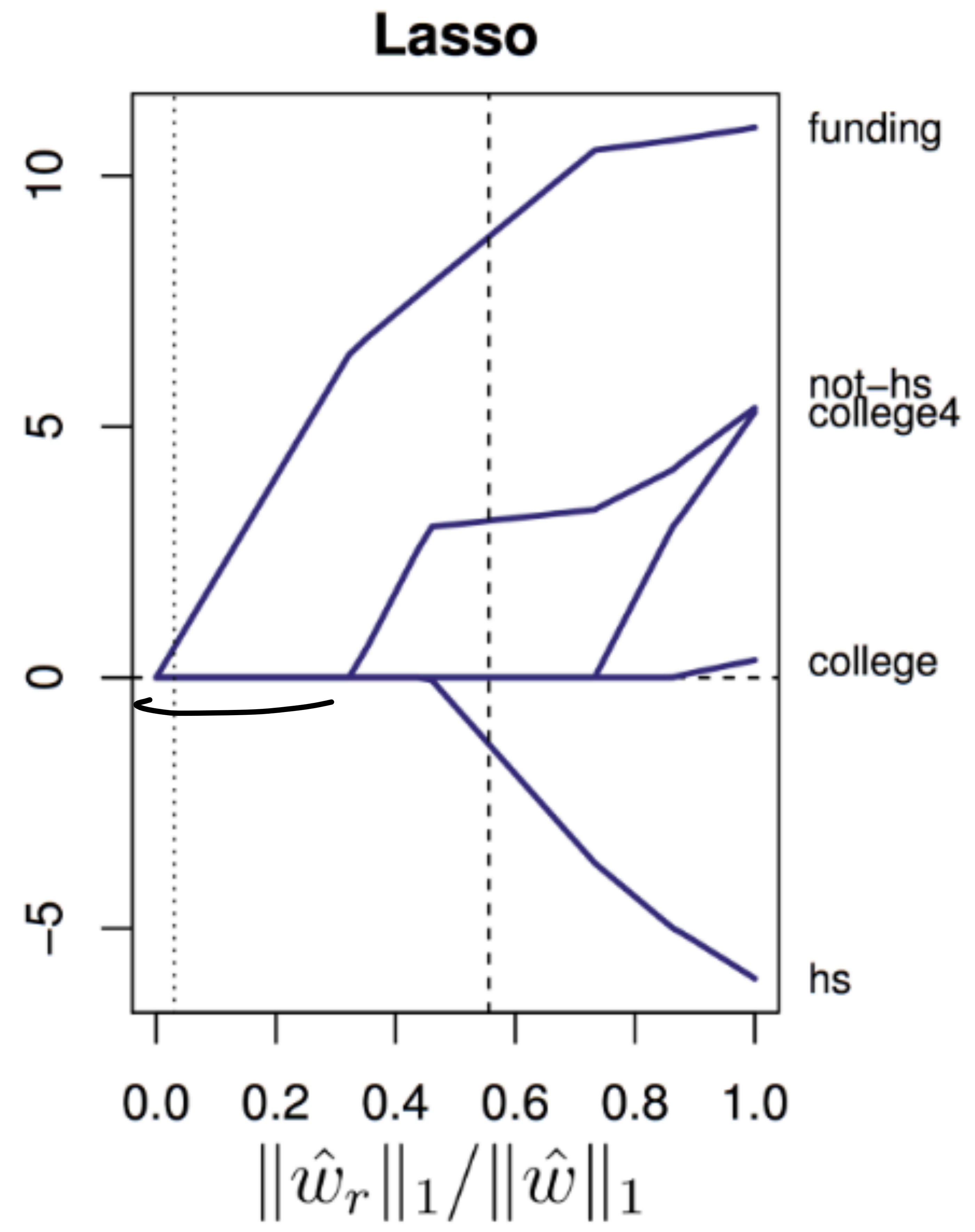
Regularization Path Comparison

$$\hat{w}_r \in \arg\min_{\|w\|_1 \le r} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

$$\hat{w} \in \arg\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

For $r = 0$, $\|\hat{w}_r\|_1 / \|\hat{w}\|_1 = 0$.

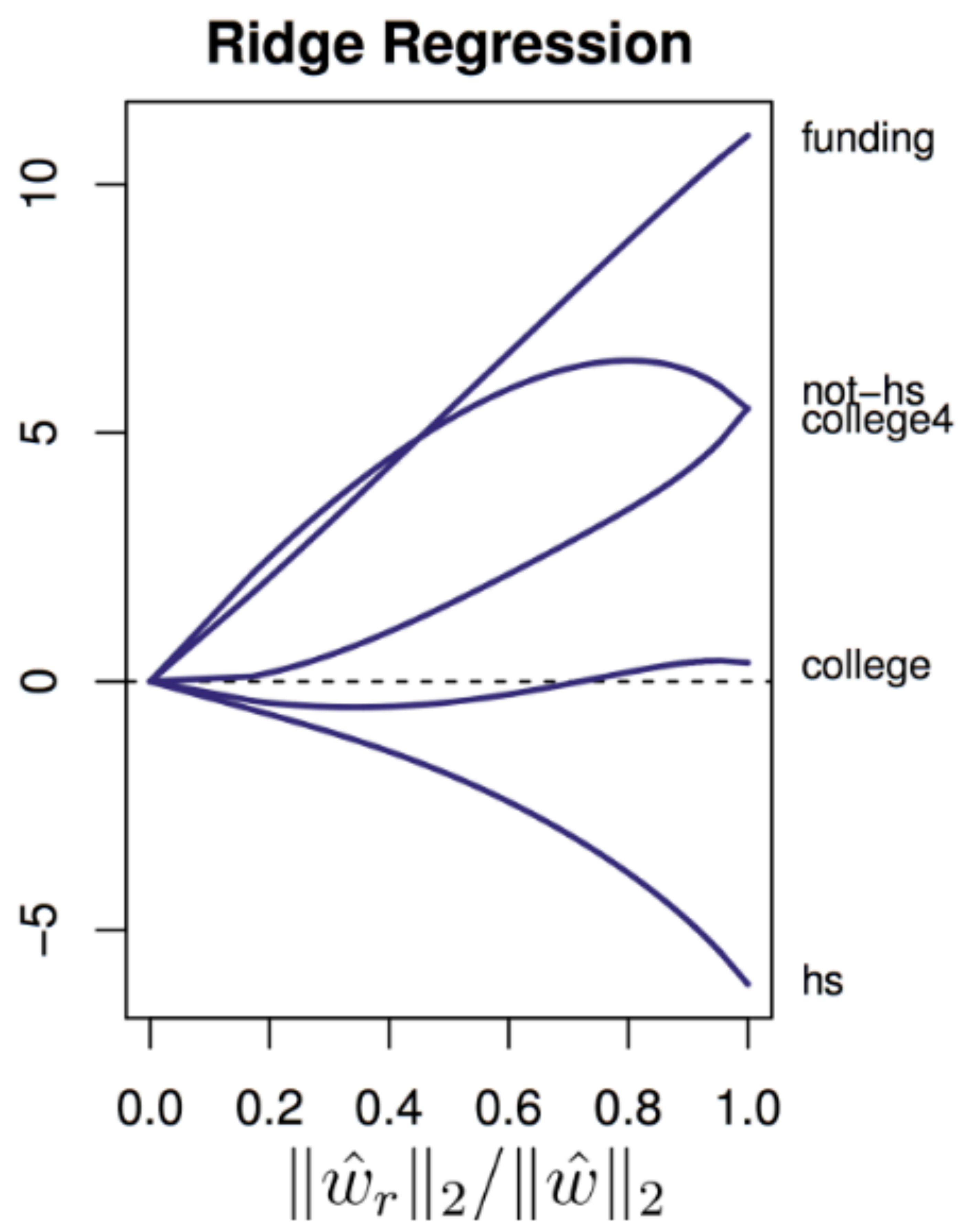
For $r = \infty$, $\|\hat{w}_r\|_1 / \|\hat{w}\|_1 = 1$.

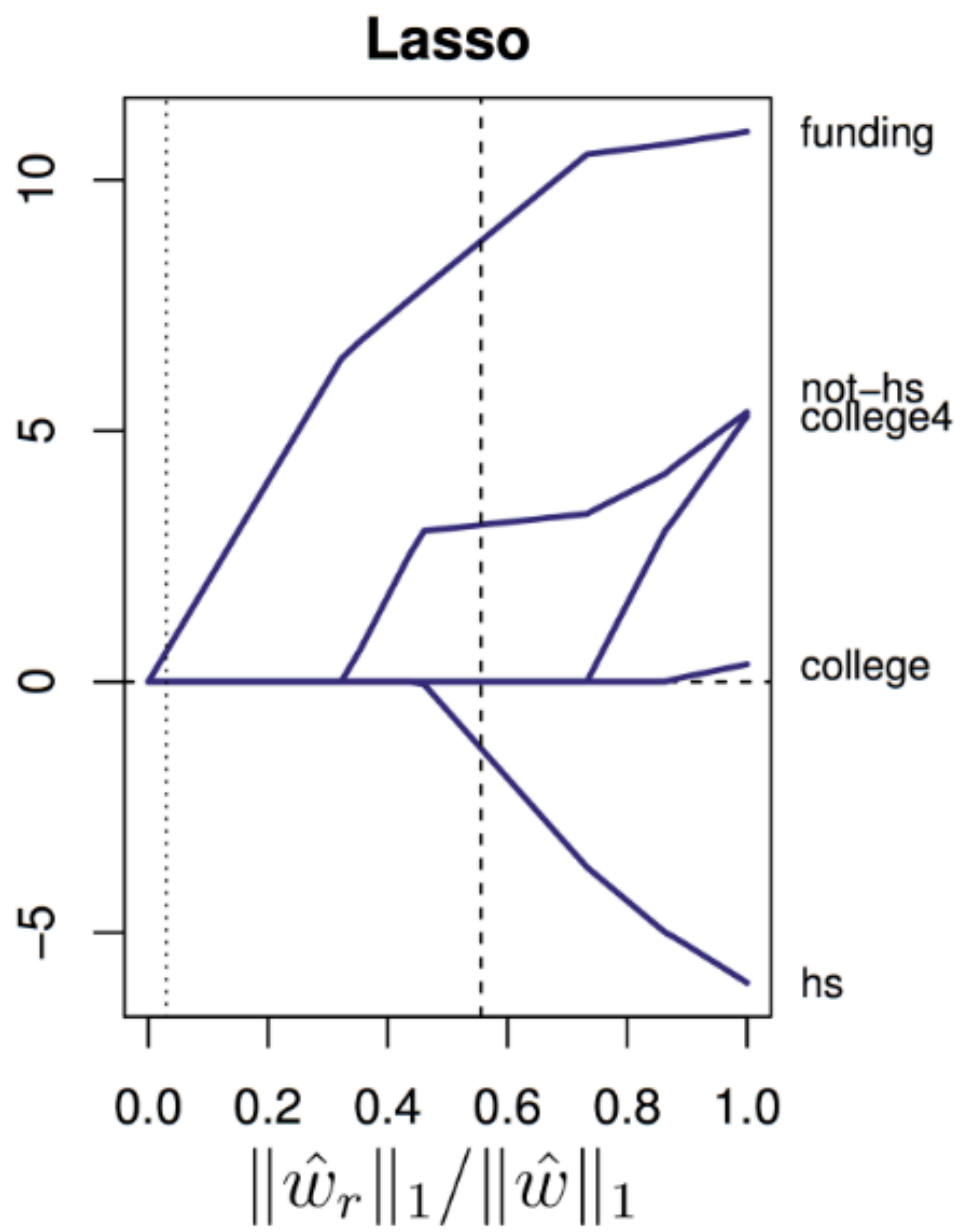


Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

Lasso vs. Ridge

Regularization Path Comparison





Lasso Regression

Pros and Cons

$$w = (\underset{=}{\overset{0}{\overset{\uparrow}{w_1}}}, \overset{0}{\overset{\uparrow}{w_2}}, \ldots, w_d)$$

Pros:

Output weights are *sparse* which can mean a more interpretable model.

More intuitive reduction in model complexity.

$$\hat{w} = (X^T X)^{-1} X^T y$$

Cons:

No closed form solution because $\|w\|_1$ is not differentiable (unlike ridge regression).

Can solve Lasso with iterative methods, but generally not as quickly as ridge regression.

Outline

Lasso Regression

Benefits of Sparsity

A **sparse** solution $\hat{w}$ is one in which many entries are 0. Why is this useful?

Faster to compute features; cheaper to measure or annotate them.

Less memory to store features (deployment on mobile device).

Interpretability: identifies the important features.

Prediction function may **generalize** better (model is less complex, i.e. $\mathscr{H}$ is “smaller”).

Parameter Space

Intuition

$w \in \mathbb{R}^2$

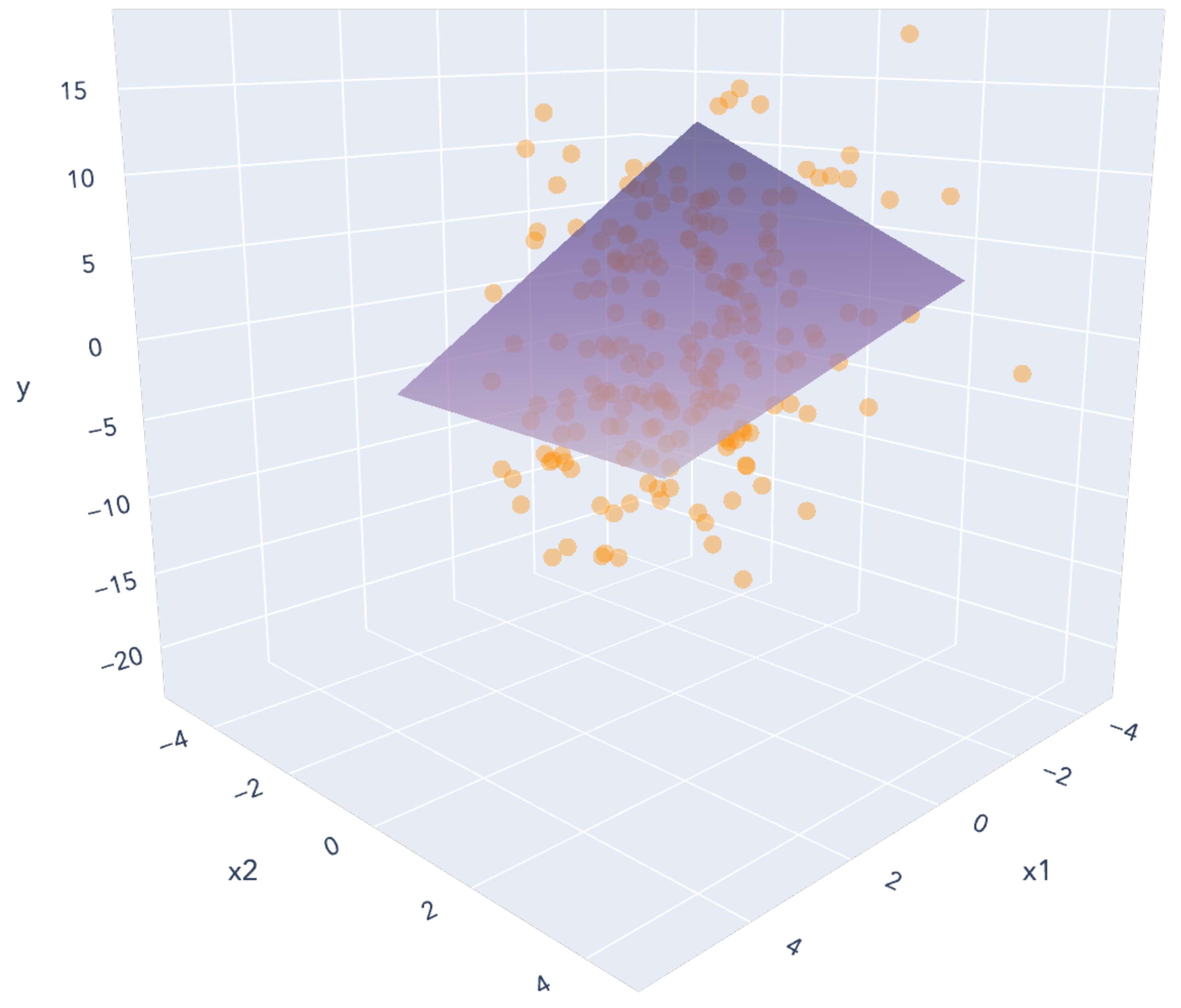
To visualize, suppose $\mathcal{X} = \mathbb{R}^2$.

$$\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2$$

Geometrically,

$w^\top x = \underline{w_1} x_1 + \underline{w_2} x_2$ is a plane through the origin in $\mathbb{R}^3$.

$\hat{R}_n(w) : \mathbb{R}^2 \to \mathbb{R}$ is a loss surface in $\mathbb{R}^3$ for every possible plane.



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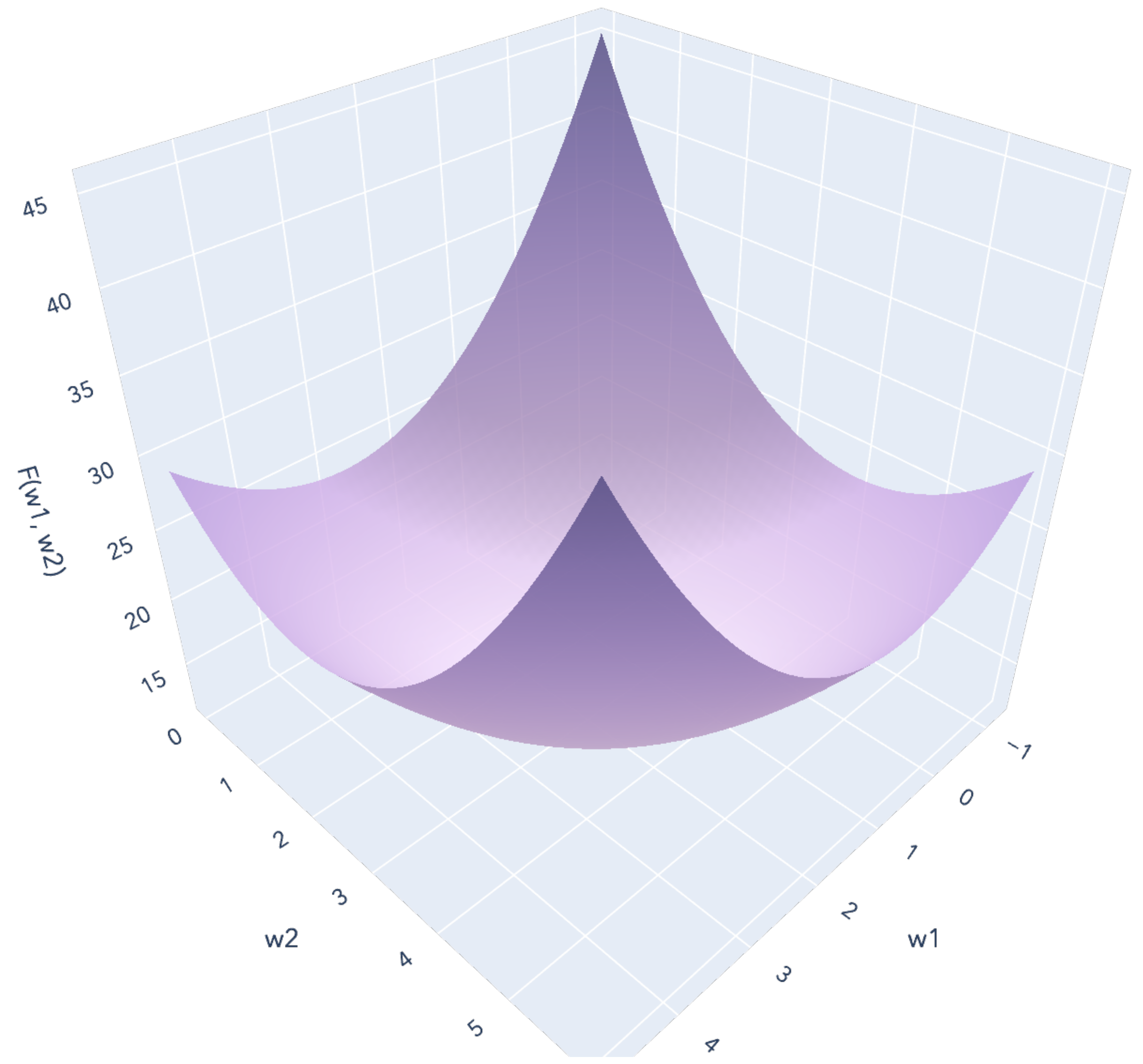

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Intuition

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$$\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2$$

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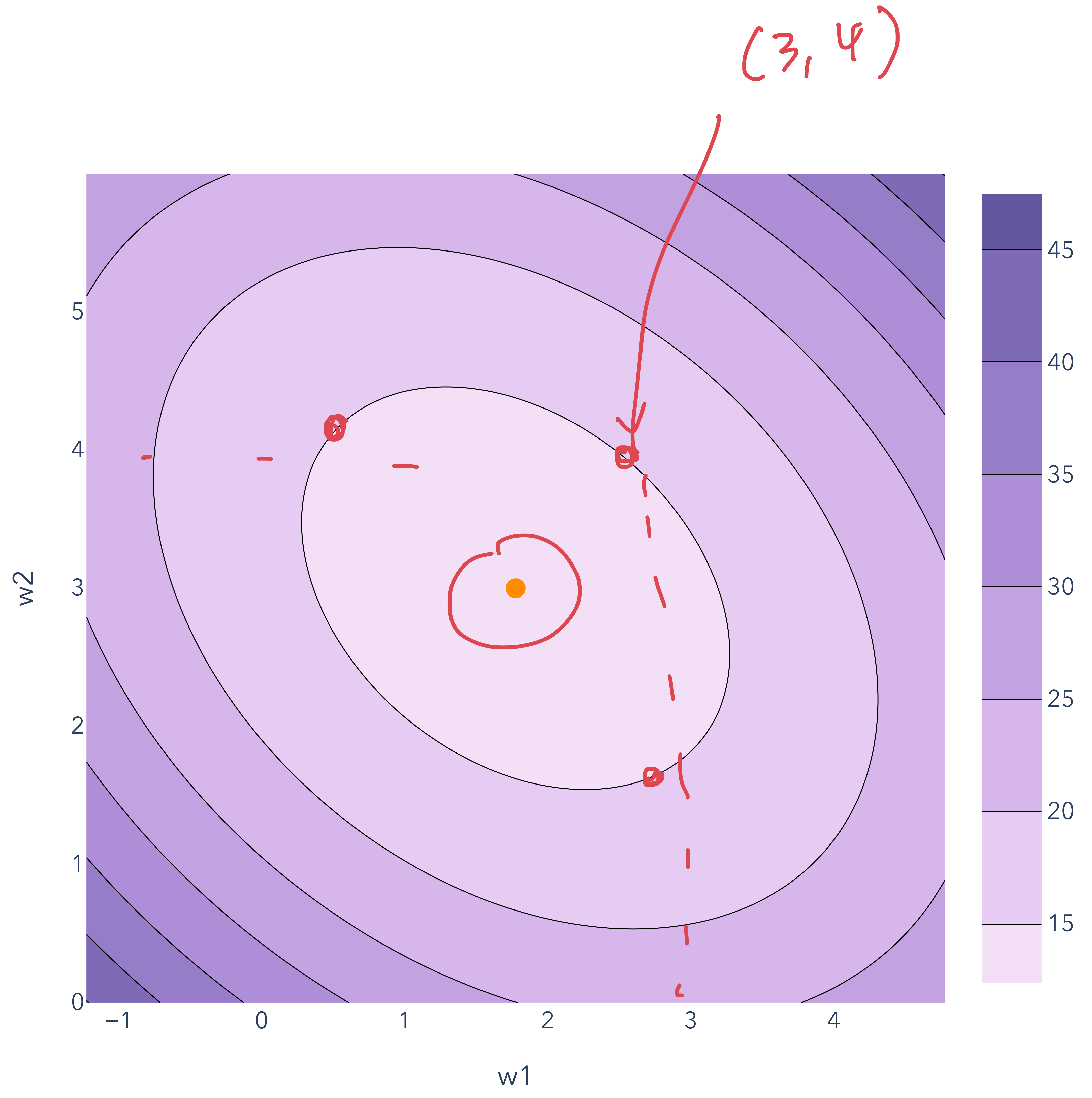


ℓ_1 and ℓ_2 Constraints

Intuition

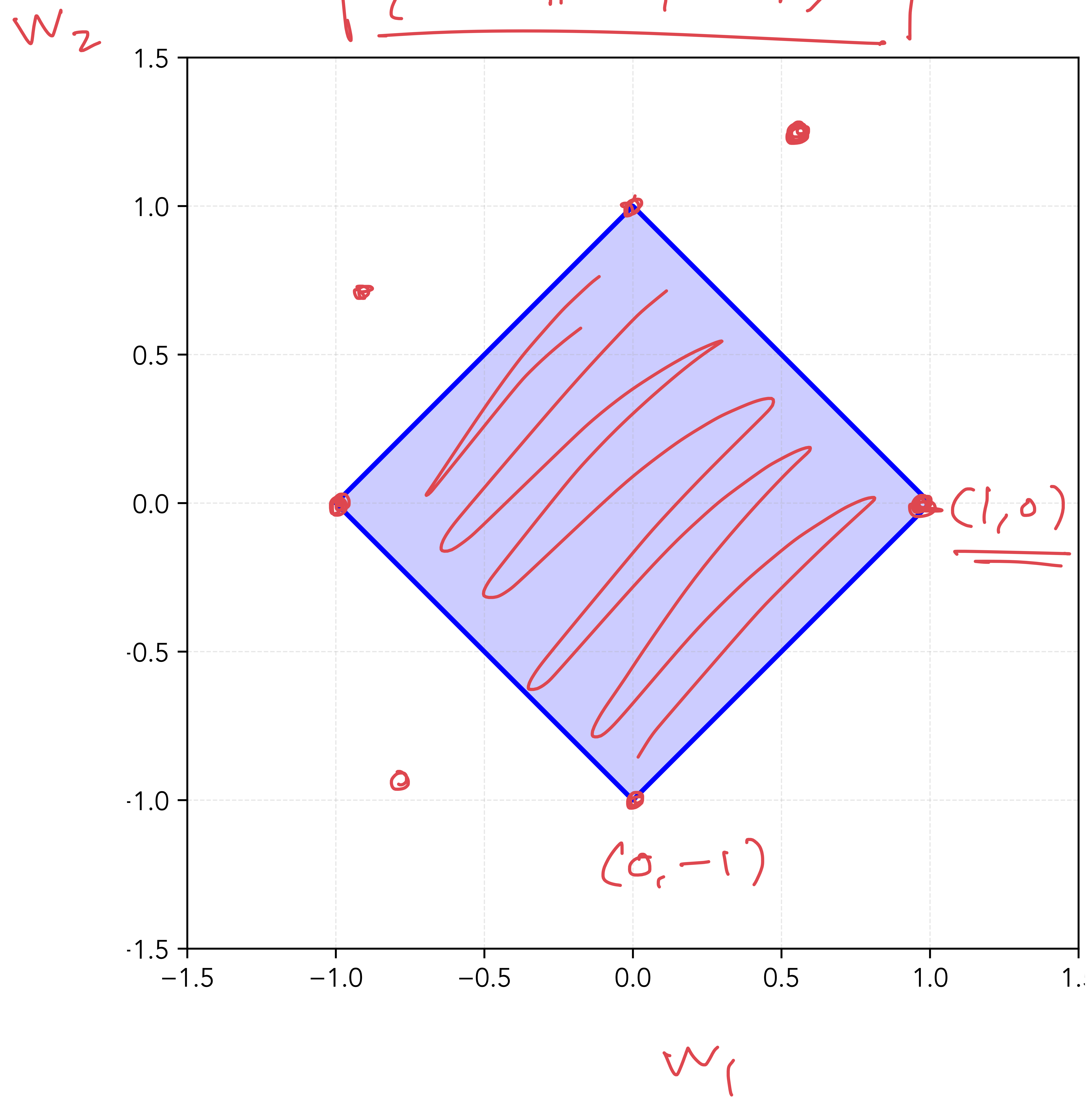
For visualization, restrict to:

$$\mathscr{H} = \{h(x) = w_1x_1 + w_2x_2\}$$

Represent $\mathscr{H}$ by $\{(w_1, w_2) \in \mathbb{R}^2\}$.

Where are the **sparse** solutions?

$\boxed{\{w : \|w\|_1 \le 1\}}$



ℓ_1 and ℓ_2 Constraints

Intuition

For visualization, restrict to:

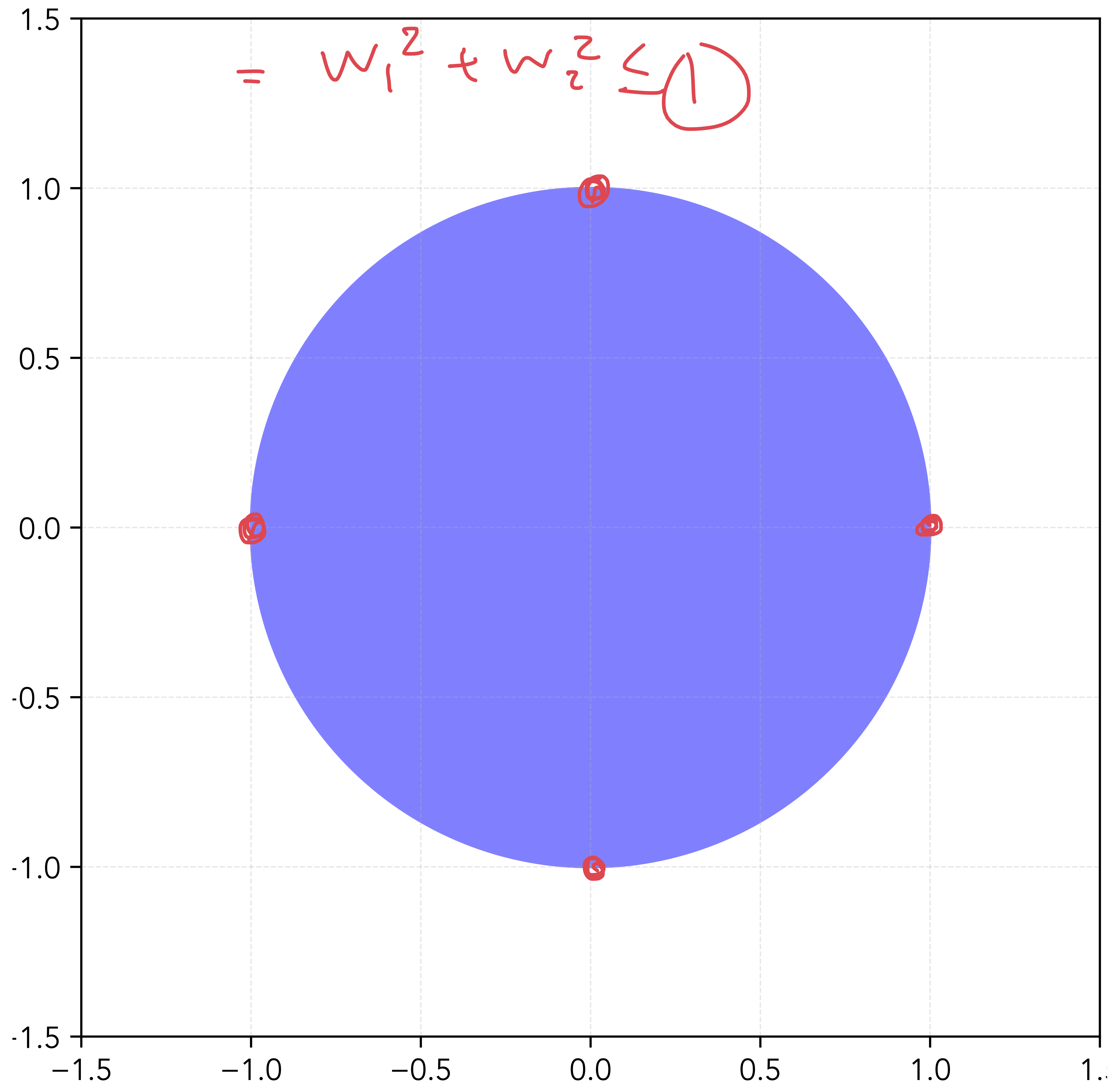
$$\mathscr{H} = \{h(x) = w_1x_1 + w_2x_2\}$$

Represent $\mathscr{H}$ by $\{(w_1, w_2) \in \mathbb{R}^2\}$.

Where are the **sparse** solutions?

$\{w : \|w\|_2 \le 1\}$.

$= w_1^2 + w_2^2 \le 1$



Empirical Risk in $\mathbb{R}^2$

Visualization for Square Loss

In matrix form: $\hat{R}_n(w) = \frac{1}{n}\|Xw - y\|^2$.

Minimizer: $\hat{w} = (X^\top X)^{-1}X^\top y$

For any $w \in \mathbb{R}^d$, by "completing square":

$$\hat{R}_n(w) = \frac{1}{n}(w - \hat{w})^\top (X^\top X)(w - \hat{w}) + \hat{R}_n(\hat{w})$$

Minimizer

The w such that $\hat{R}_n(w)$ exceeds $\hat{R}_n(\hat{w})$ by $c > 0$ are ellipsoids centered at $\hat{w}$:

$$\left\{w : \hat{R}_n(w) = c + \hat{R}_n(\hat{w})\right\} = \left\{w : (w - \hat{w})^\top X^\top X(w - \hat{w}) = nc\right\}$$

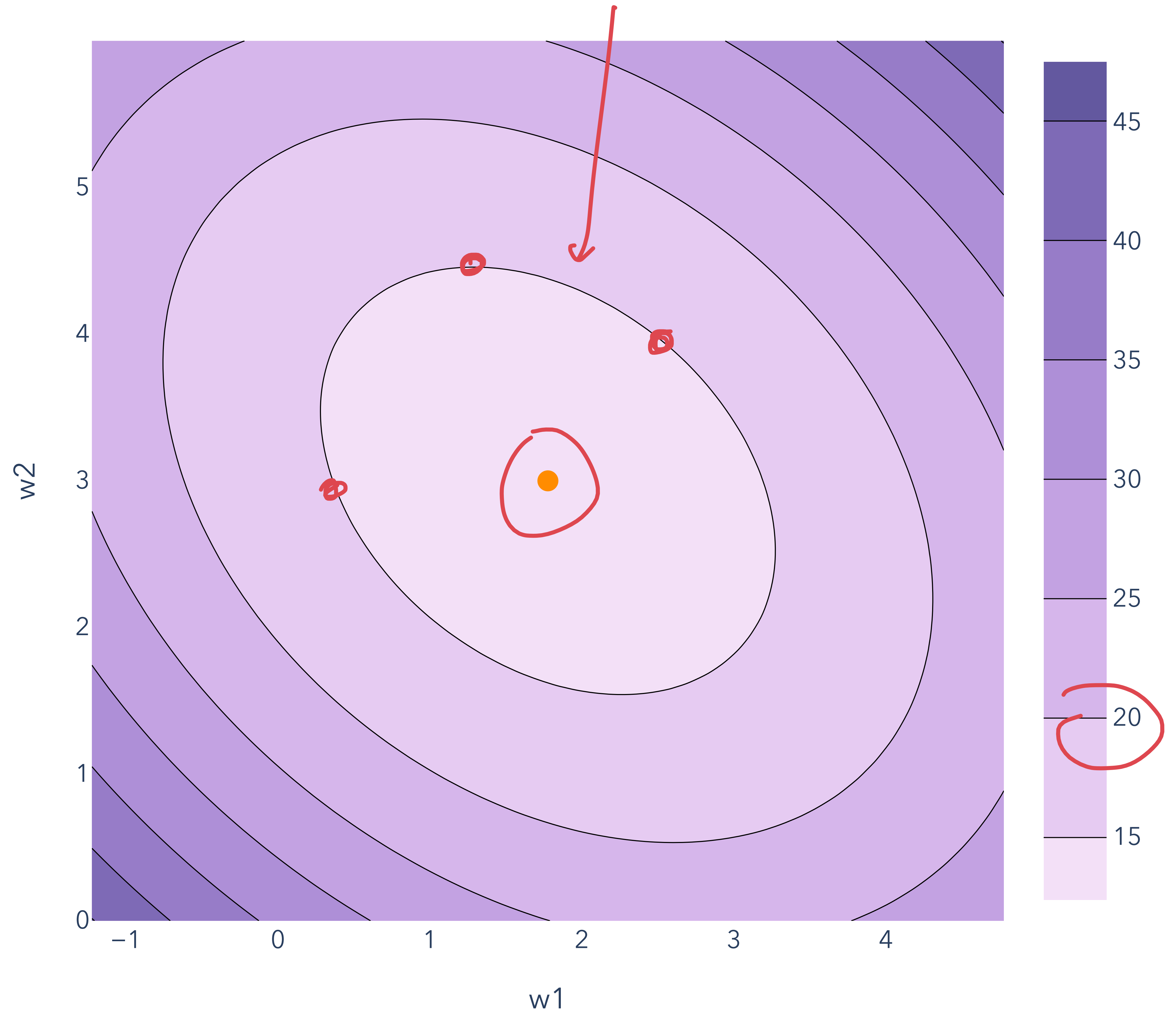
Empirical Risk in $\mathbb{R}^2$

Visualization for Square Loss

The w such that $\hat{R}_n(w)$ exceeds $\hat{R}_n(\hat{w})$ by $c > 0$ are ellipsoids centered at $\hat{w}$:

$$\left\{ w : \hat{R}_n(w) = c + \hat{R}_n(\hat{w}) \right\}$$

$$= \left\{ w : (w - \hat{w})^\top X^\top X (w - \hat{w}) = nc \right\}$$



ℓ_1 Regularization

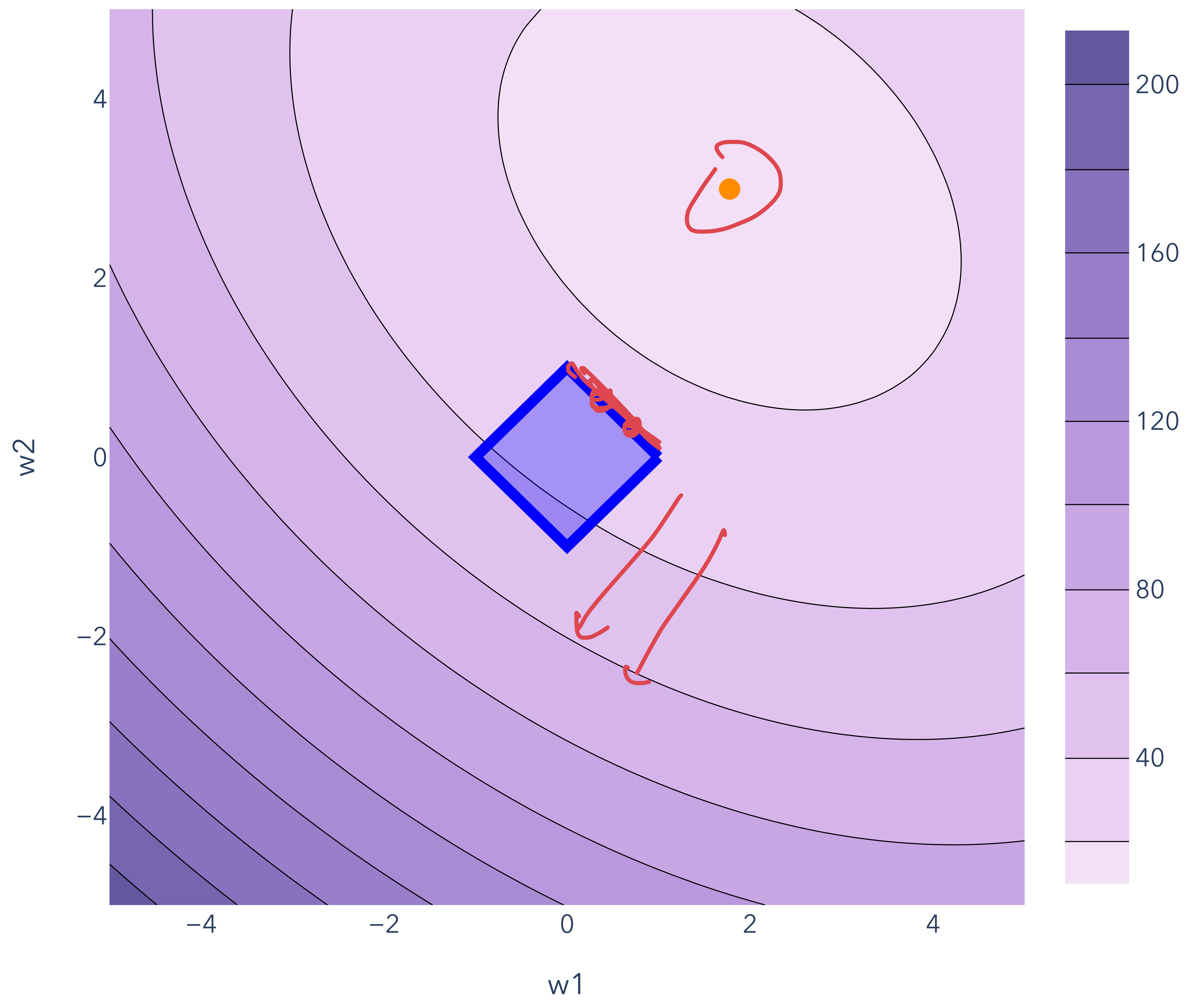
Visualization

$\hat{R}_n(w)$

$$\hat{w}_r \in \arg\min_{w \in \mathbb{R}^2} \underline{\frac{1}{n}\sum_{i=1}^{n}(w^\top x^{(i)} - y^{(i)})^2}$$

subject to: $|w_1| + |w_2| \le r = 1$

$\|w\|_1 \le 1$

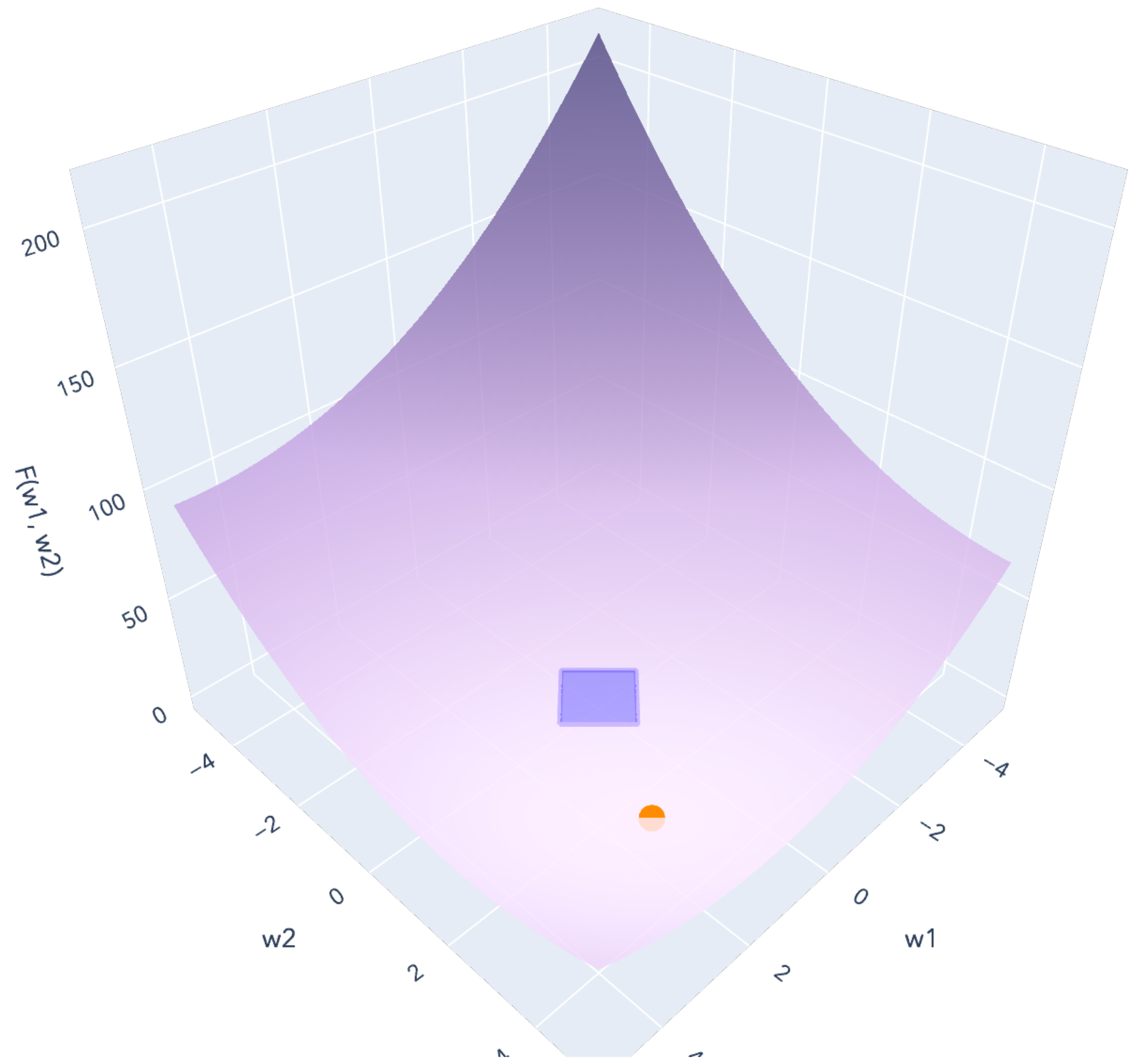


ℓ_1 Regularization

Visualization

$$\hat{w}_r \in \underset{w \in \mathbb{R}^2}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

$$\text{subject to: } \left|w_1\right| + \left|w_2\right| \leq r$$

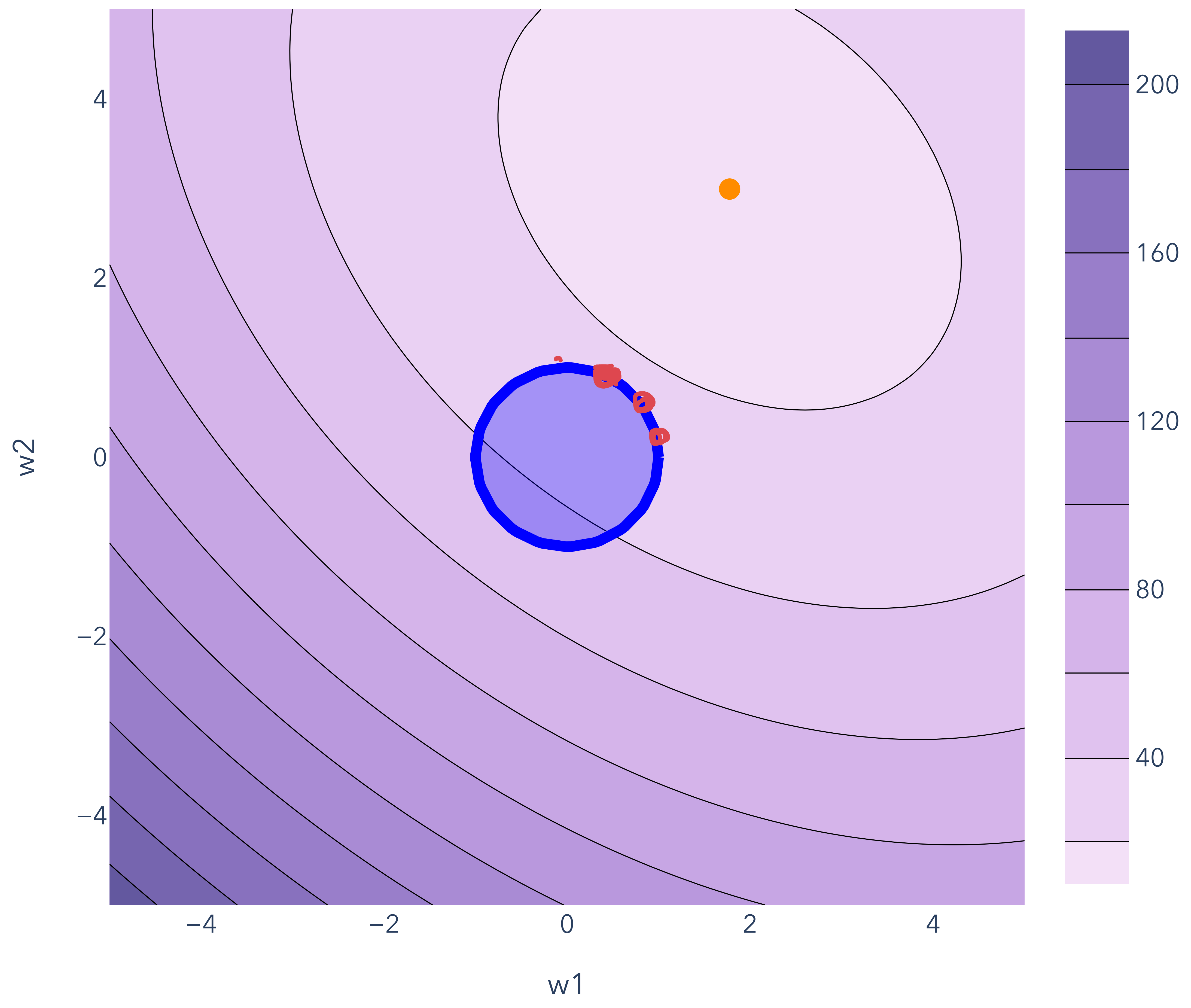


ℓ_2 Regularization

Visualization

$$\hat{w}_r \in \arg\min_{w \in \mathbb{R}^2} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

$$\text{subject to: } w_1^2 + w_2^2 \leq r$$

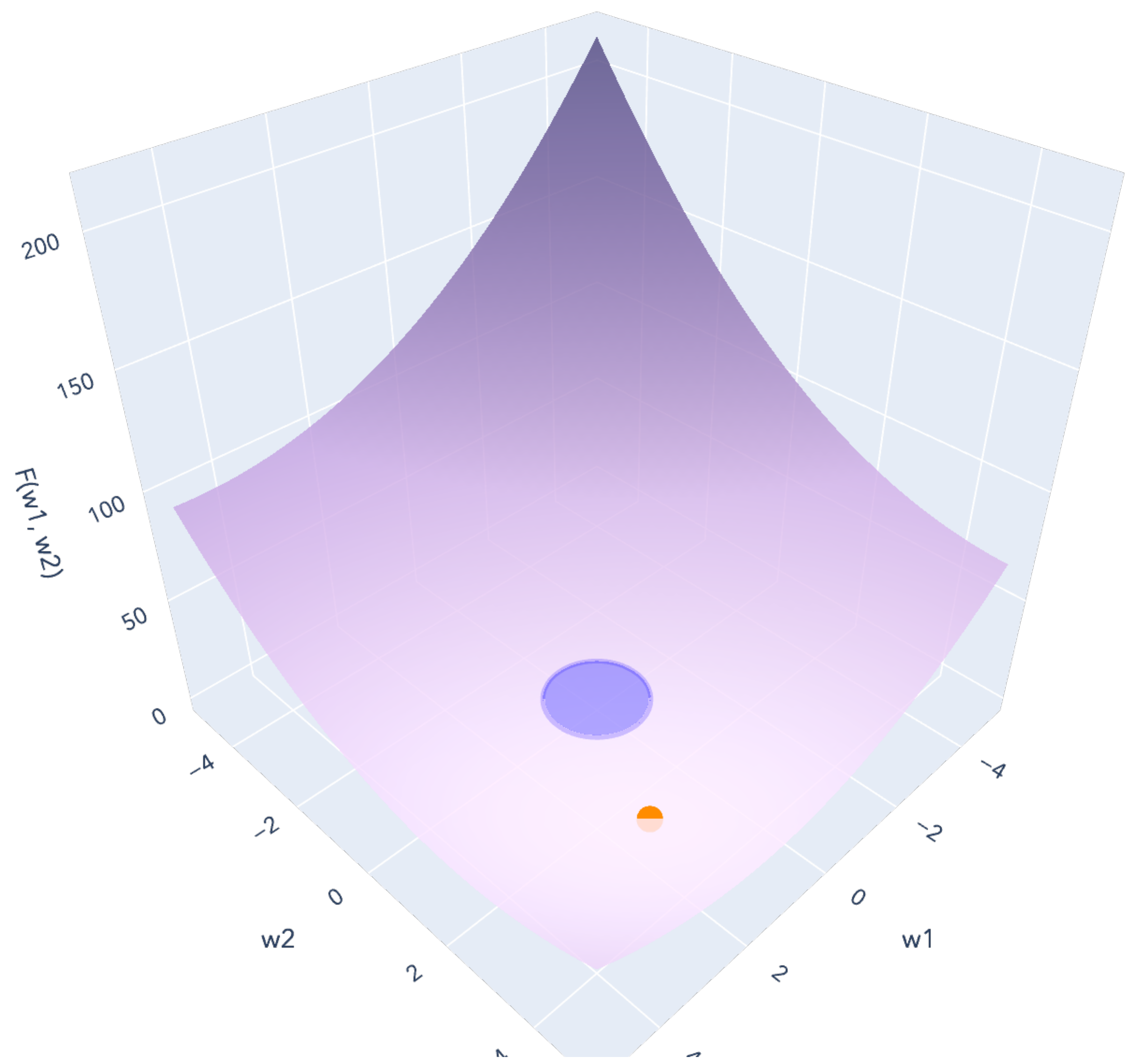


ℓ_2 Regularization

Visualization

$$\hat{w}_r \in \arg\min_{w \in \mathbb{R}^2} \frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2$$

subject to: $\underline{\underline{w_1^2 + w_2^2 \leq r}}$



Sparsity

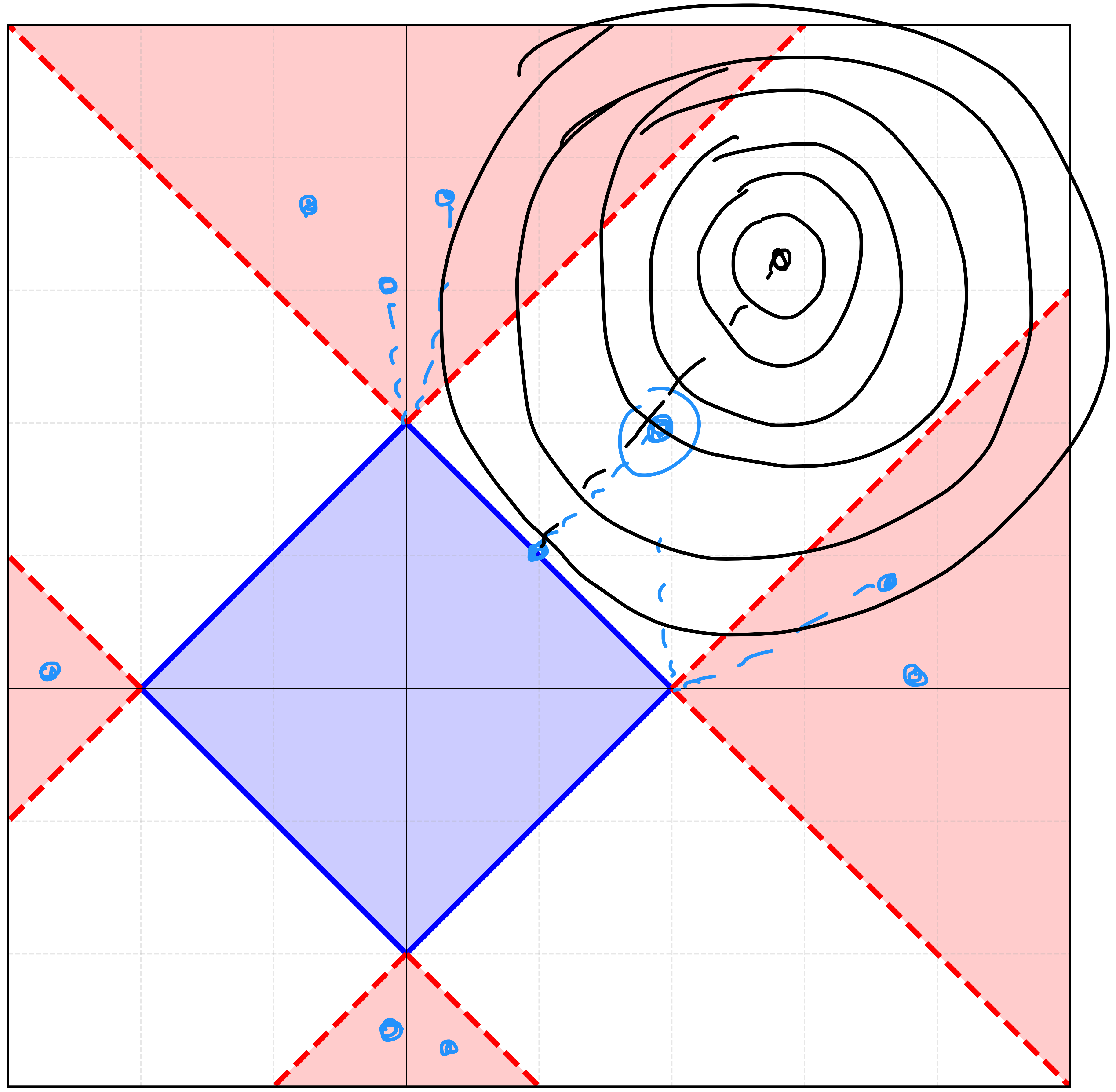
Geometric Intuition

Suppose $\underline{X^\top X = I}$ (orthogonal features).

Then, contours are perfect circles.

The $\hat{w}$ in red regions are closest to corners in the ℓ_1 ball.

Geometric intuition: Projection onto diamond (ℓ_1 ball) encourages solutions at corners.



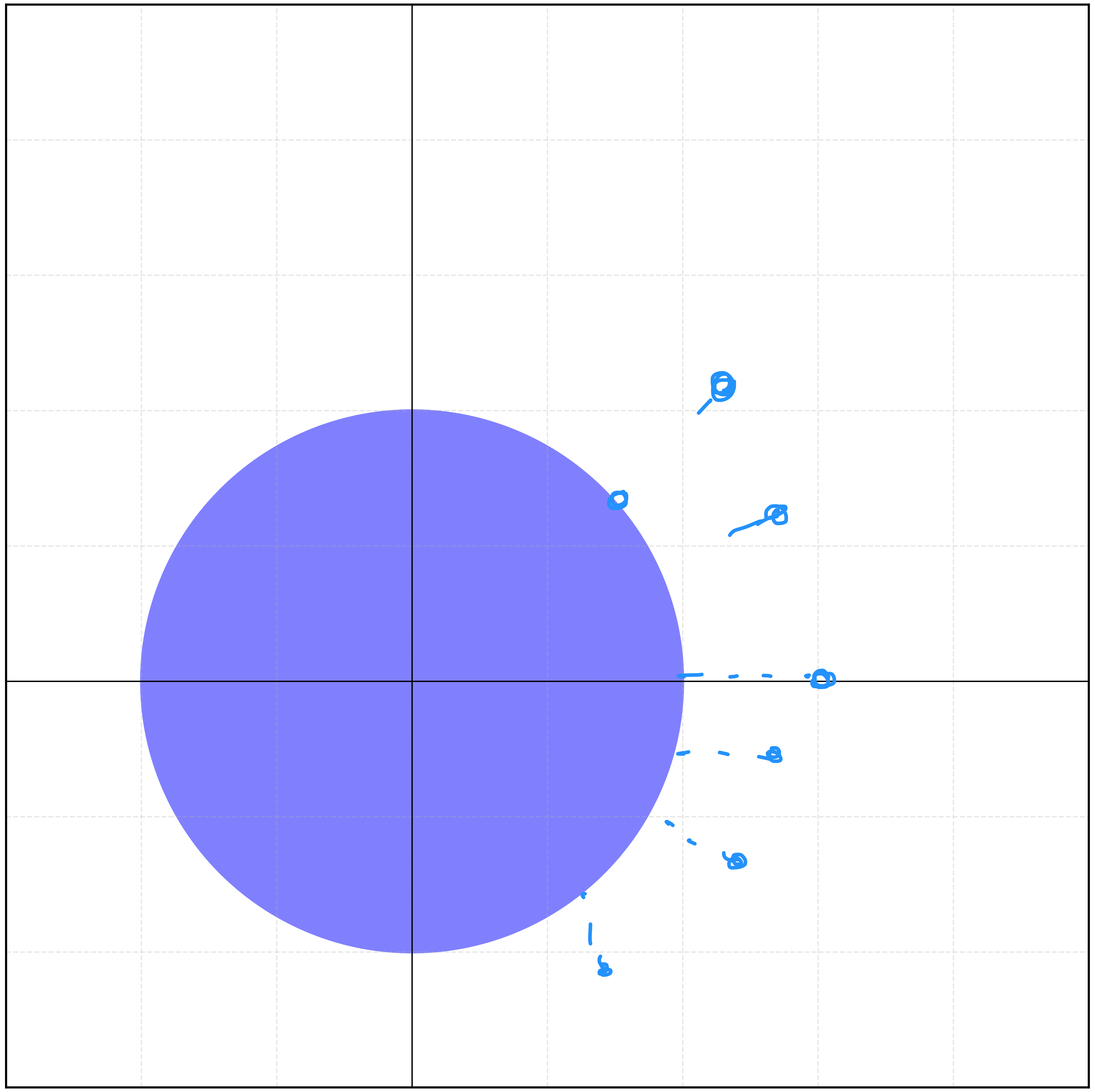
Sparsity

Geometric Intuition

Suppose $X^\top X = I$ (orthogonal features).

Then, contours are perfect circles.

Geometric intuition: Projection onto sphere (ℓ_2 ball) encourages solutions equally.



ℓ_q Regularization

Geometric Intuition

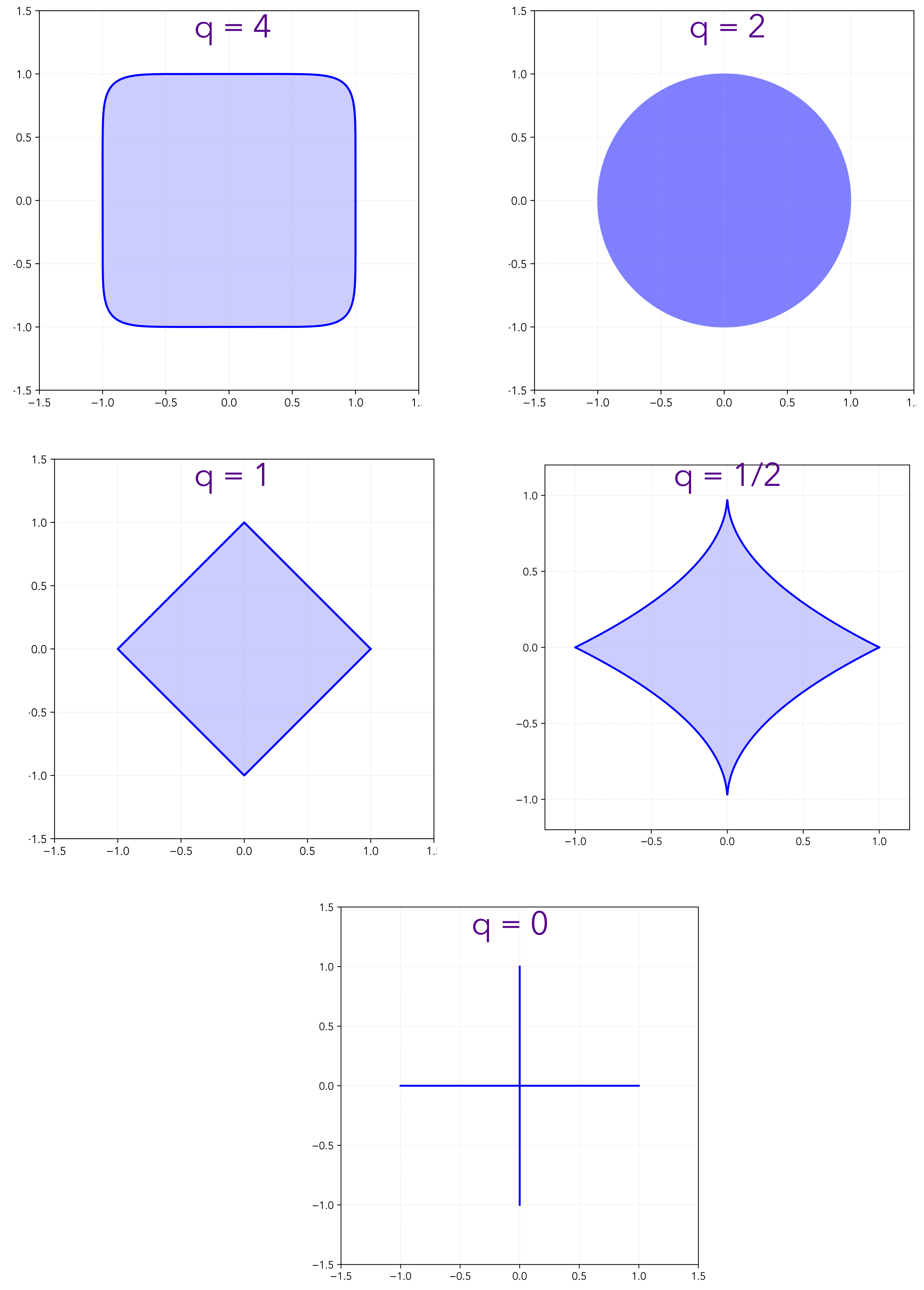
Generalize to ℓ_q:

$$\underline{(\|w\|_q)^q} = |w_1|^q + |w_2|^q$$

Note: $\|w\|_q$ is only a norm for $q \geq 1$ but not for $q \in (0,1)$.

When $q < 1$, the ℓ_q constraint is non-convex (so hard to optimize).

ℓ_0 defined as number of non-zero weights, i.e. subset selection.



$W = (\overset{0}{\overset{\shortparallel}{w_1}}, \overset{0}{\overset{\shortparallel}{\ldots}}, \ldots, \overset{0}{\overset{\shortparallel}{w_d}})$

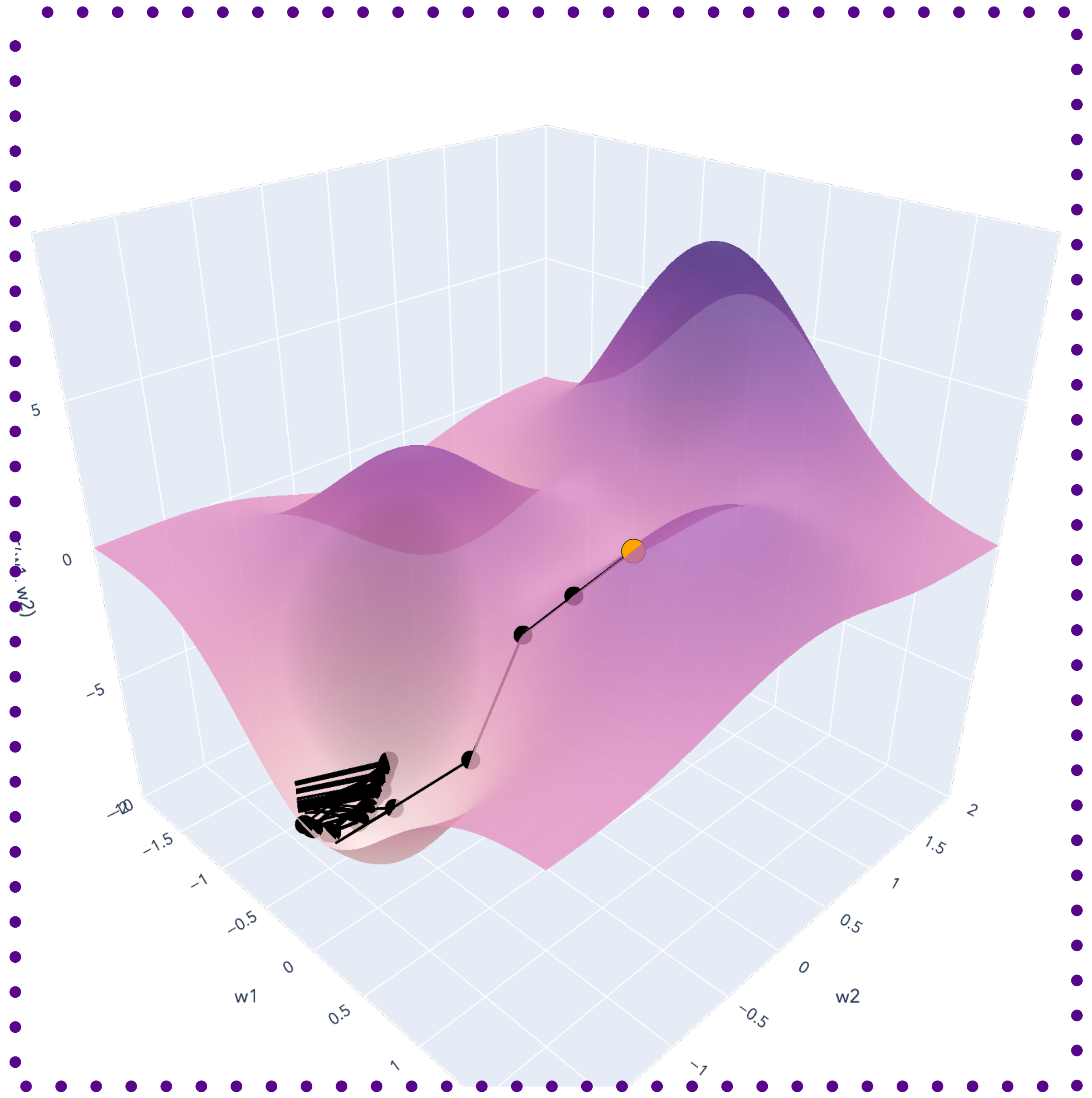
Other Forms of Regularization

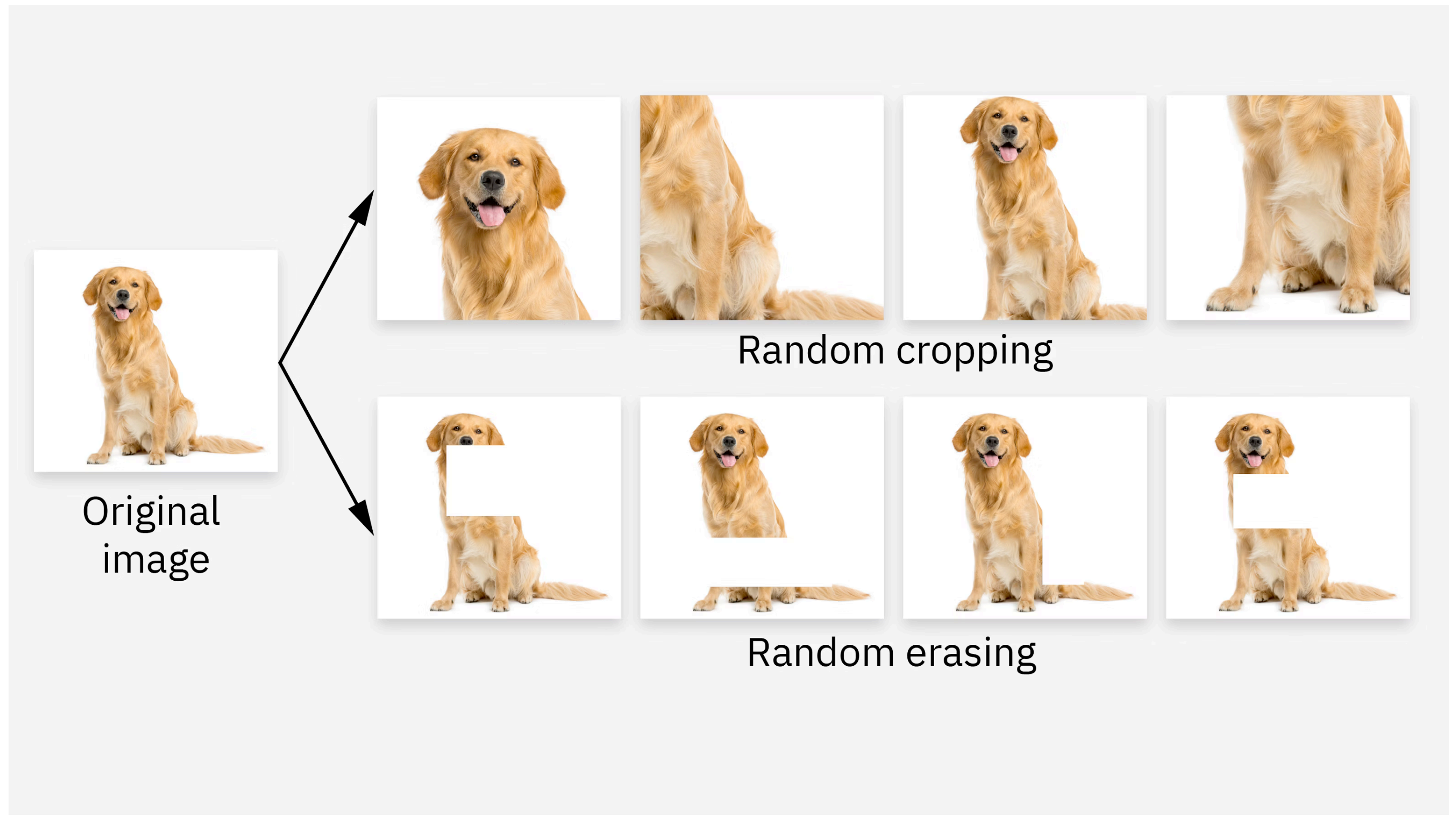
Implicit Regularization, Weight Decay, etc.

In general, regularization is a term that describes ways to "bias" a problem with infinitely many solutions to a smaller subset of solutions.

Implicit regularization. Properties of the optimization algorithm lead to "simple" solutions.

Data augmentation. Randomly modify training data in by an operation, usually used in deep learning (e.g. randomly cropping images).





Outline

Regression

Problem Instance

Input space: $\mathscr{X} = \mathbb{R}^d$

Action space: $\mathscr{A} = \mathbb{R}$

Outcome space: $\mathscr{Y} = \mathbb{R}$

$\hat{y}$ is the predicted value (the **action**).

y is the observed value (the **outcome**).

Distance Based Loss

Definition

In general, loss functions take the form:

$$(\hat{y}, y) \mapsto \ell(\hat{y}, y) \in \mathbb{R}$$

Regression losses typically depend on the residual $r = y - \hat{y}$.

A loss function is distance-based if:

1. It only depends on the residual: $\ell(\hat{y}, y) = \psi(y - \hat{y})$ for some $\psi : \mathbb{R} \to \mathbb{R}$
2. It is zero when the residual is zero: $\psi(0) = 0$.

Loss Functions

Examples

$$r = y - \hat{y}$$

Square (ℓ_2) loss: $\ell(r) = r^2$.

Absolute (ℓ_1) loss: $\ell(r) = |r|$.

Outliers typically have large residuals.

Square loss more affected by outliers than absolute loss.

y	$\hat{y}$	$y - \hat{y}$	$(y - \hat{y})^2$
1	0	1	1
5	0	5	25
10	0	10	100
50	0	50	2500

Loss Functions

Examples

$$r = y - \hat{y}$$

Square (ℓ_2) loss: $\ell(r) = r^2$.

Absolute loss: $\ell(r) = |r|$.

Outliers typically have large residuals.

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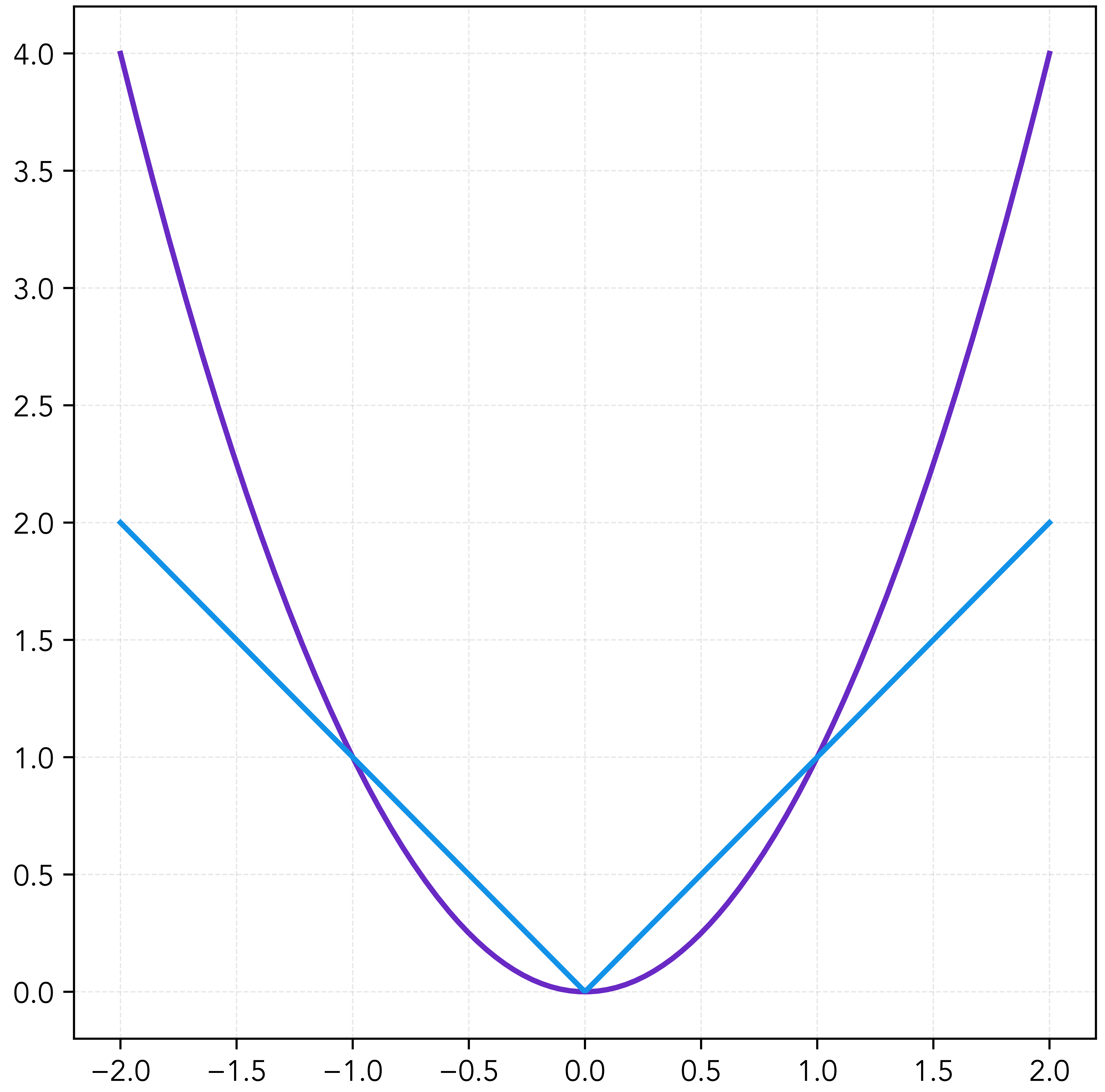


Loss Functions

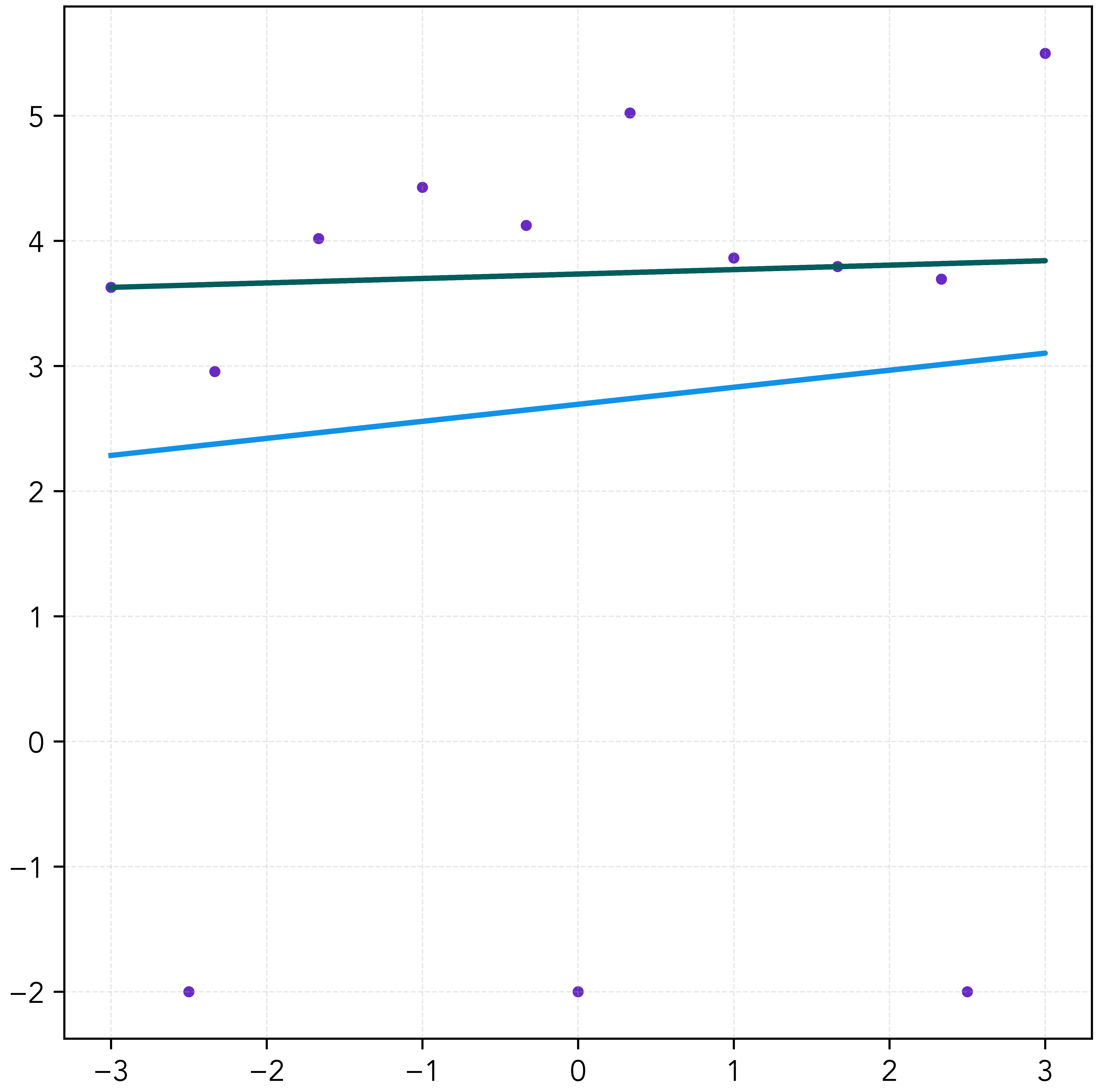
Robustness

$$r = y - \hat{y}$$

Square (ℓ_2) loss: $\ell(r) = r^2$.

Absolute loss: $\ell(r) = |r|$.

Robustness refers to how affected a learning algorithm is by outliers.



Loss Functions

Robustness

Square loss: $\ell(r) = r^2$

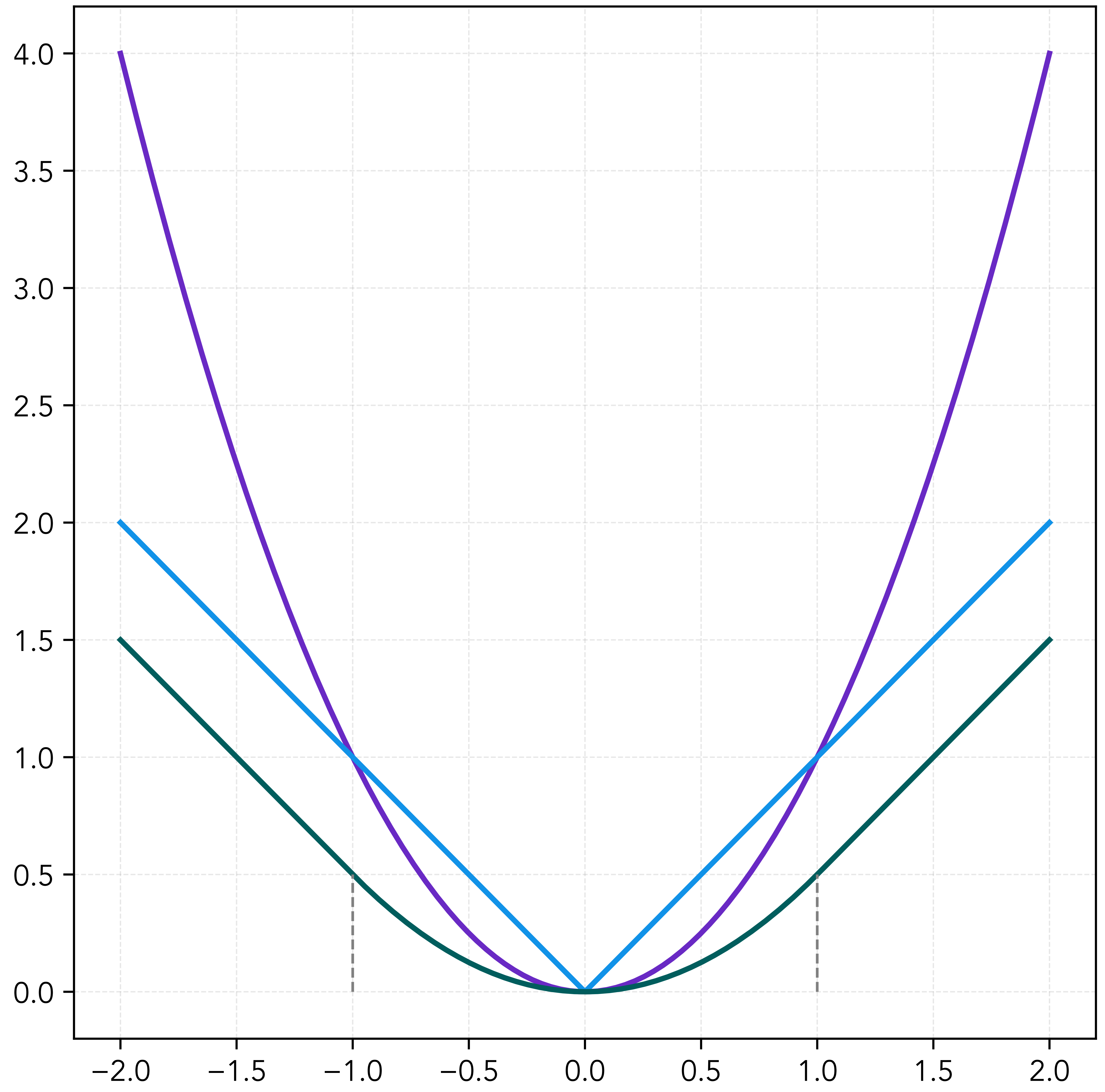
(not robust)

Absolute loss: $\ell(r) = |r|$

(not differentiable)

Huber loss: Quadratic for $|r| \le \delta$ and linear for $|r| > \delta$

(robust and differentiable)



Outline

Classification

Problem Instance

Input space: $\mathcal{X} = \mathbb{R}^d$

Action space: $\mathcal{A} = \{-1,1\}$

Outcome space: $\mathcal{Y} = \{-1,1\}$

We've already seen the zero-one loss for $f : \mathcal{X} \to \{-1,1\}$:

$$\ell(f(x), y) = \mathbf{1}\{f(x) \neq y\}$$

But let's allow real-valued predictions $f : \mathcal{X} \to \mathbb{R}$.

Classification

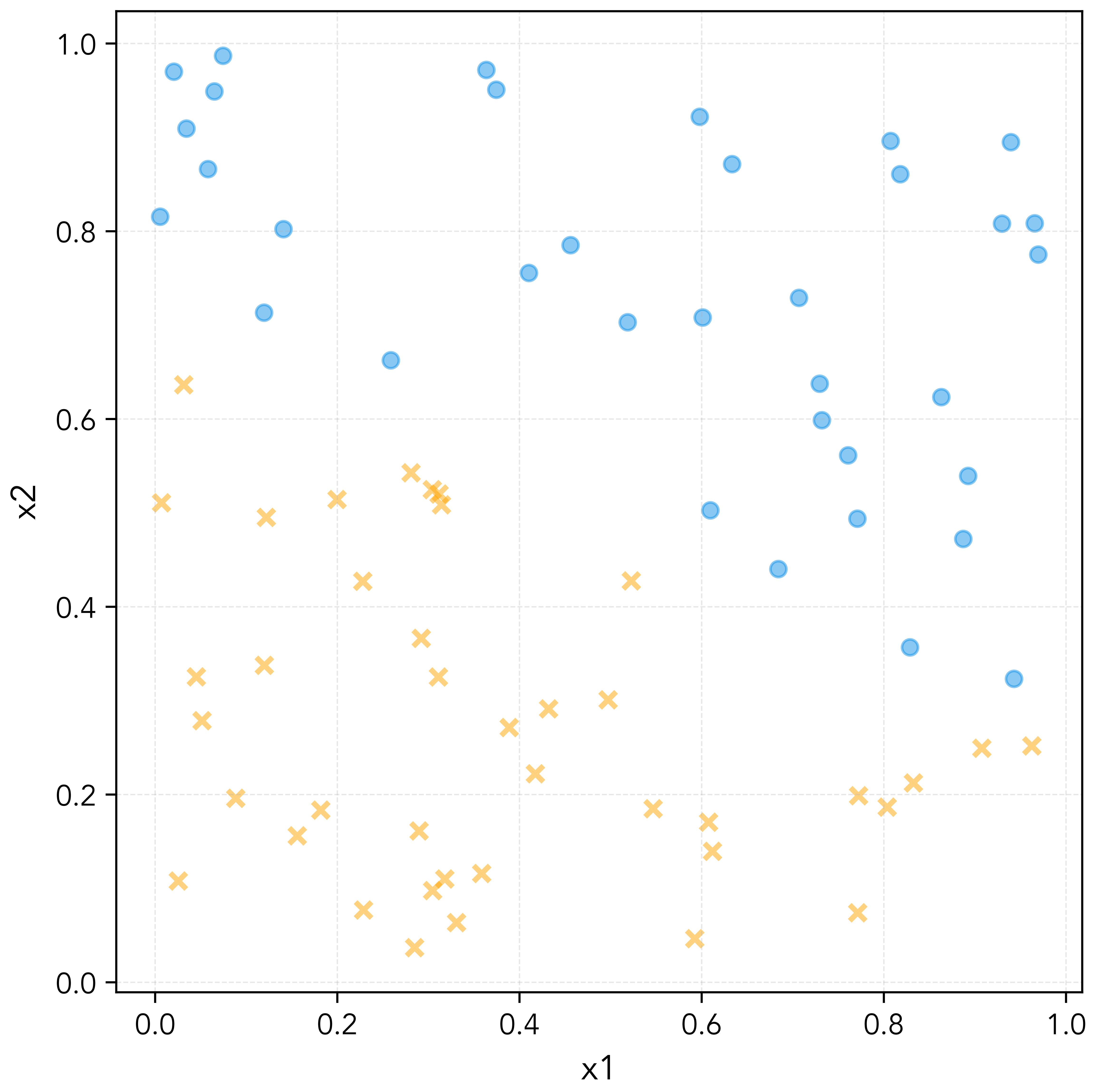
Geometric Picture

Input space: $\mathcal{X} = \mathbb{R}^d$

Action space: $\mathcal{A} = \{-1, 1\}$

Outcome space: $\mathcal{Y} = \{-1, 1\}$

Geometrically: find a **decision boundary** between the classes.



Classification

Geometric Picture

Input space: $\mathscr{X} = \mathbb{R}^d$

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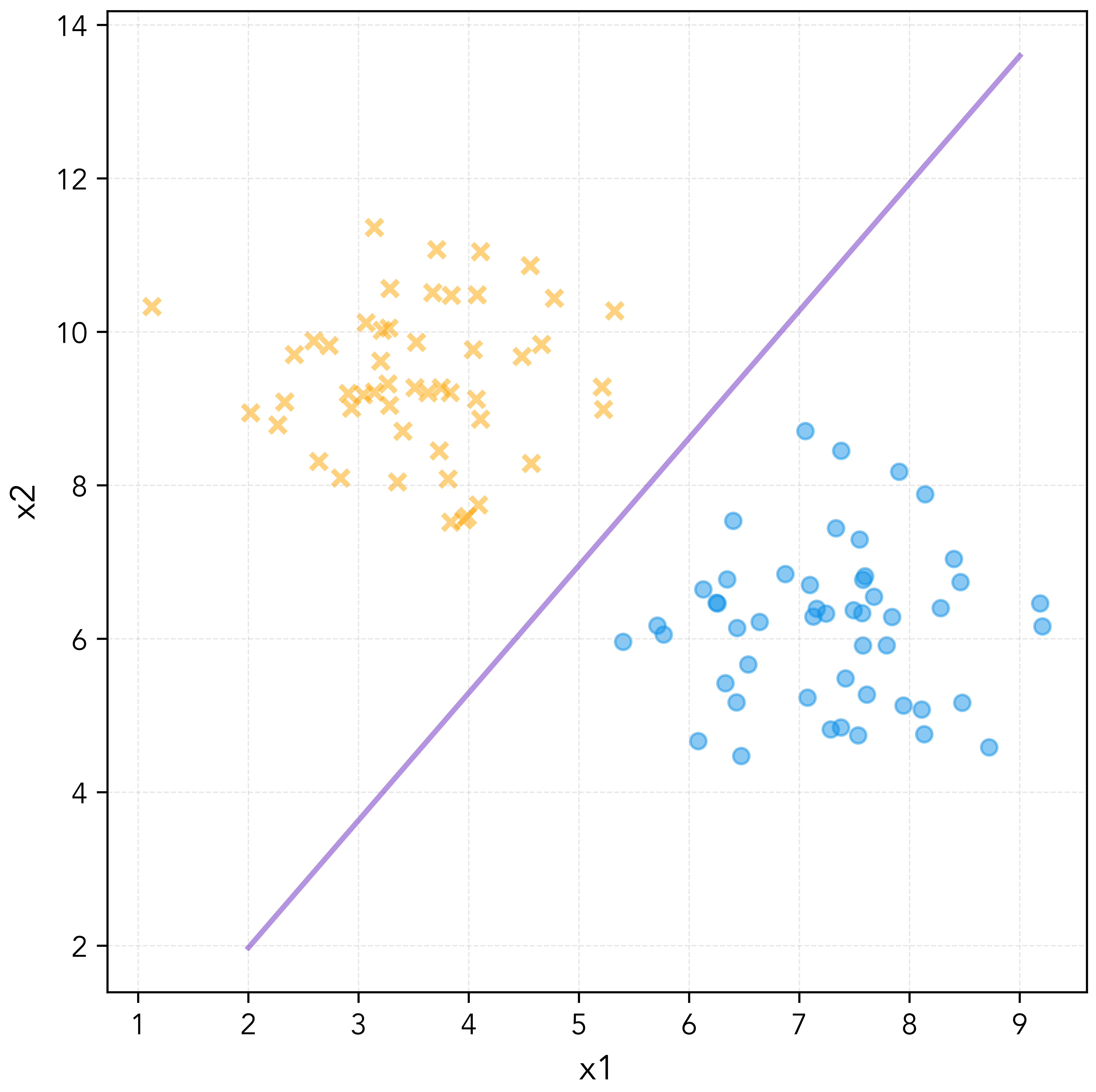
We will focus on methods that induce **linear decision boundaries.**



Classification

Geometric Picture

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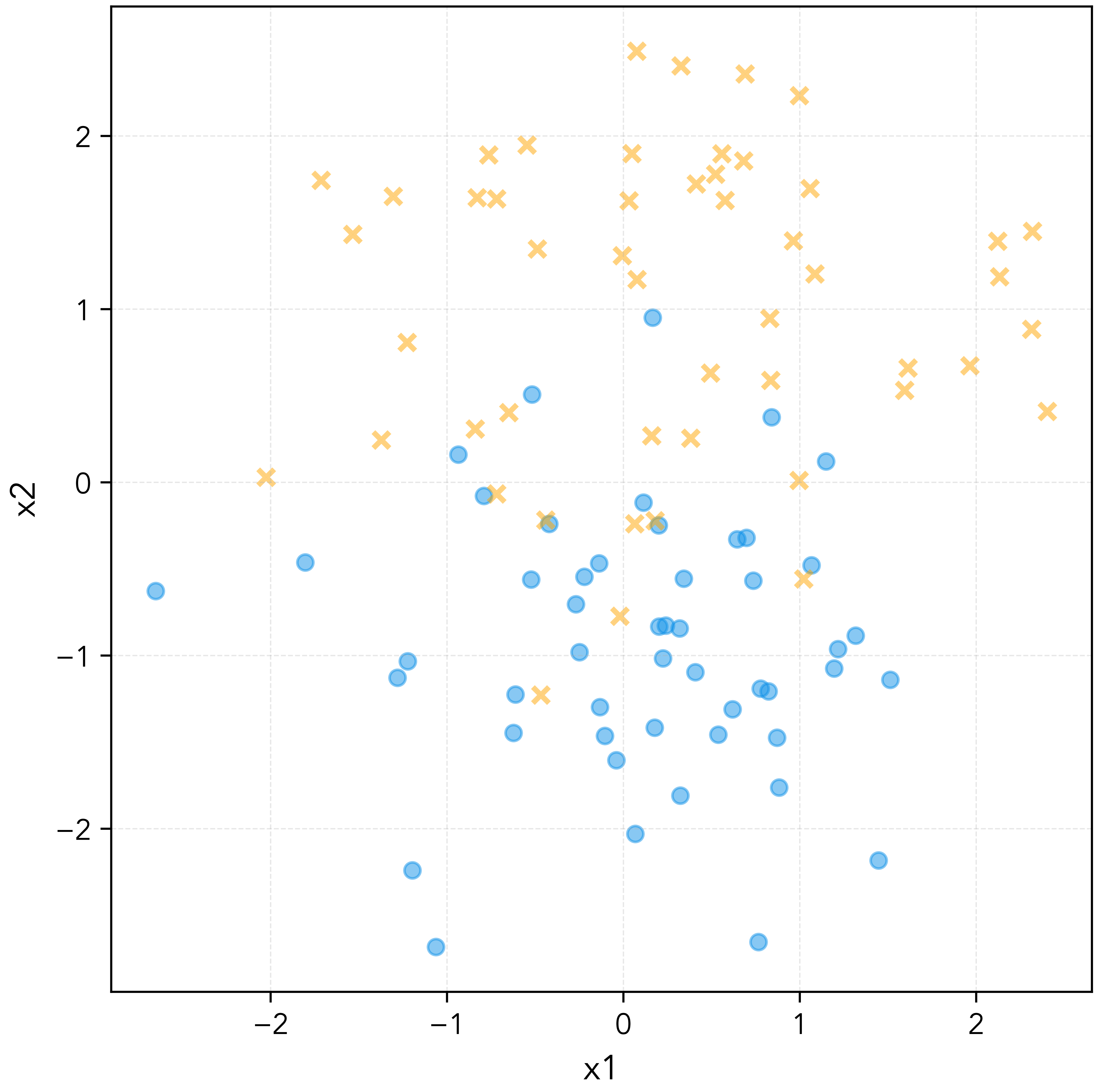
Outcome space: $\mathscr{Y} = \{-1,1\}$

We will focus on methods that induce **linear decision boundaries.**

Most problems are *not* linearly separable (i.e. there exists a hyperplane separating the $y = -1$ and $y = 1$ points).



Classification

Problem Instance

Input space: $\mathcal{X} = \mathbb{R}^d$

Action space: $\mathcal{A} = \mathbb{R}$

Outcome space: $\mathcal{Y} = \{-1, 1\}$

But let's allow real-valued predictions $f : \mathcal{X} \to \mathbb{R}$.

$$f(x) > 0 \implies \text{Predict } 1$$

$$f(x) < 0 \implies \text{Predict } -1$$

Classification

Problem Instance

Input space: $\mathcal{X} = \mathbb{R}^d$

Action space: $\mathcal{A} = \mathbb{R}$

Outcome space: $\mathcal{Y} = \{-1,1\}$

For a **linear** function $f(x) = w^\top x$:

$$w^\top x > 0 \implies \text{Predict } 1$$

$$w^\top x < 0 \implies \text{Predict } -1$$

Classification

Score Function

Outcome space: $\mathcal{Y} = \{-1, 1\}$ Action space: $\mathcal{A} = \mathbb{R}$

For a real-valued prediction function $f : \mathcal{X} \to \mathbb{R}$, the value $f(x)$ is called the score for input x.

In this context, we can call f a **score function**.

The magnitude of the score can be interpreted as **confidence** in our prediction.

Margin

Definition

The margin for a predicted score $\hat{y}$ and the true class $y \in \{-1,1\}$ is $y\hat{y}$.

With a score function $f : \mathcal{X} \to \mathbb{R}$, the margin is $yf(x)$.

If y and $\hat{y}$ are the same sign, prediction is **correct** and margin is **positive**.

If y and $\hat{y}$ have different sign, prediction is **incorrect** and margin is **negative**.

We want to find f that **maximizes** the margin.

Many classification losses only depend on the margin (margin-based losses).

Classification Losses

Zero-One Loss

$$h(x) = \text{sign}(f(x)) := \begin{cases} 1 & \text{if } f(x) \geq 0 \\ -1 & \text{if } f(x) < 0 \end{cases}$$

The zero-one loss for $h : \mathcal{X} \to \{-1, 1\}$ is $\ell(h(x), y) = \mathbf{1}\{h(x) \neq y\}$.

We can rewrite this in terms of the margin and score function as

$$\ell(f(x), y) := \mathbf{1}\{yf(x) \leq 0\}.$$

The empirical risk for zero-one loss, given dataset D_n:

$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\{y^{(i)} f(x^{(i)}) \leq 0\}$$

Classification Losses

Zero-One Loss

The empirical risk for zero-one loss, given dataset D_n:

$$\hat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}\{y^{(i)} f(x^{(i)}) \leq 0\}$$

Non-convex, non-differentiable, and discontinuous.

Optimization problem is NP-hard (computationally infeasible).

Classification Losses

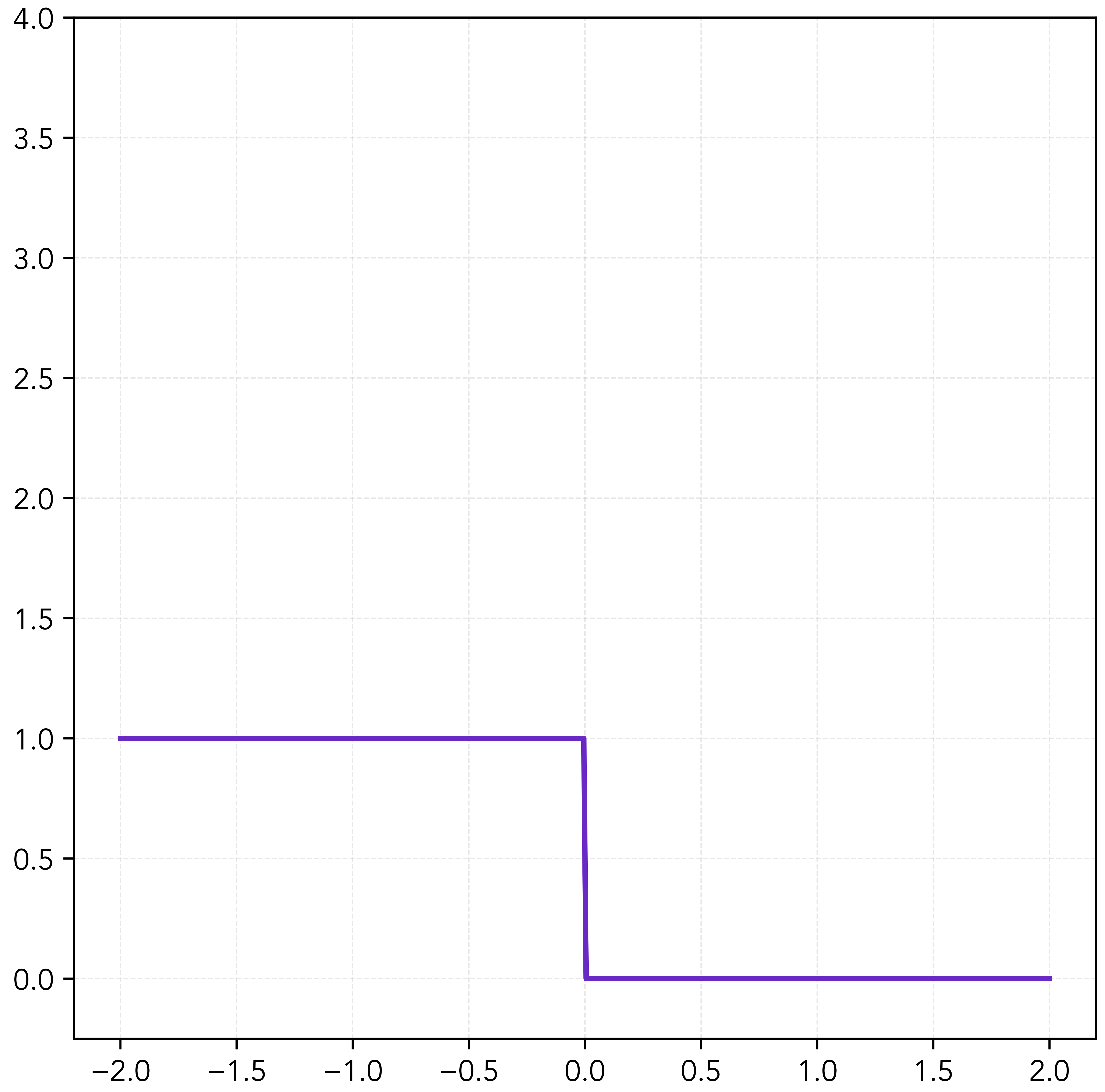
Zero-One Loss

Margin: $m = \hat{y}y$

Zero-one loss: $\ell_{0-1}(m) := \mathbf{1}\{m \leq 0\}$

x-axis is margin:

$m > 0 \iff$ classification is **correct**.



Classification Losses

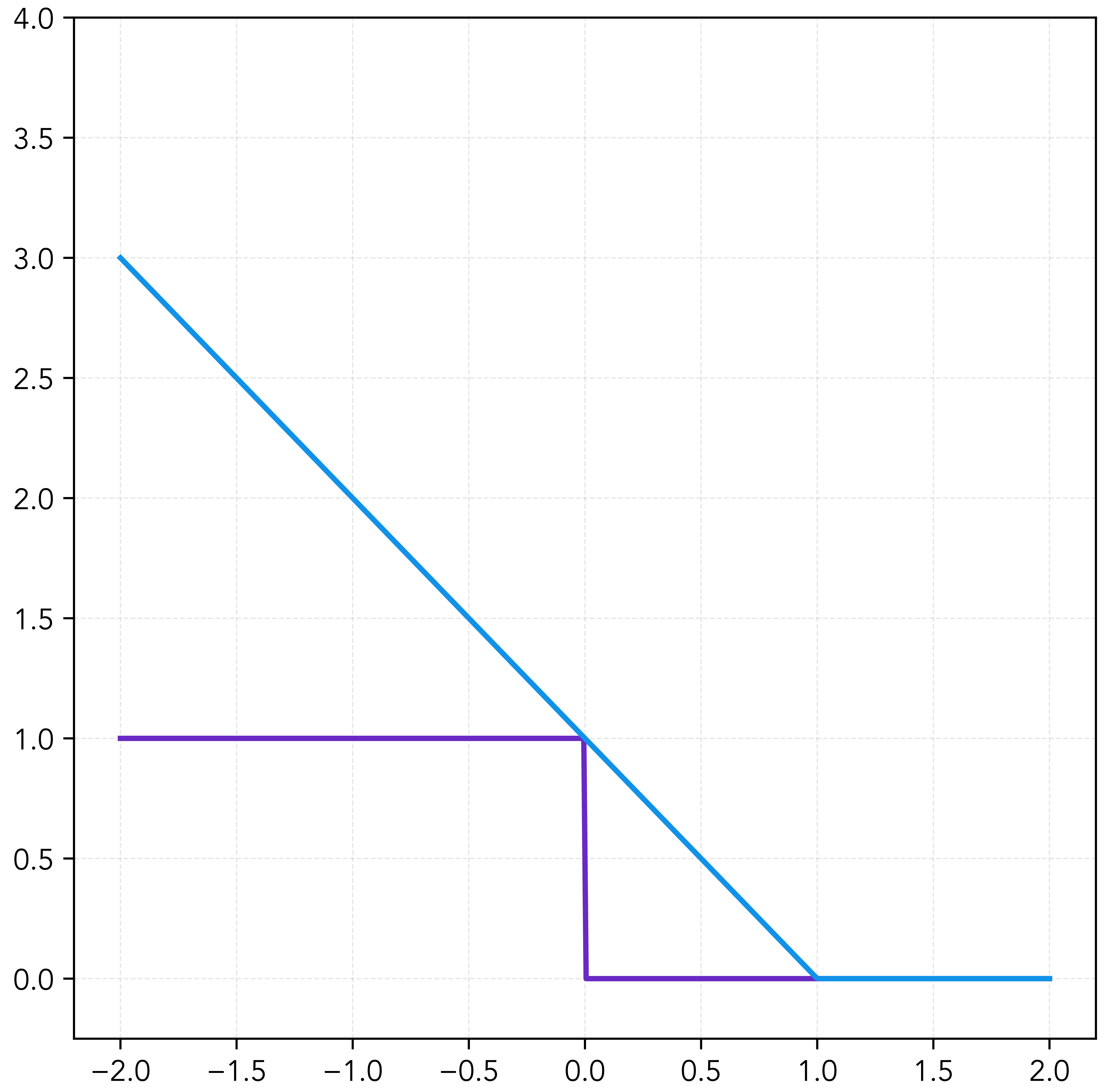
Hinge Loss

Margin: $m = \hat{y}y$

Hinge loss: $\ell_{\text{hinge}}(m) := \max(1 - m, 0)$

Hinge loss is **convex, upper bound** on zero-one loss.

Not differentiable at $m = 1$.



Hinge Loss

(Soft-Margin) Support Vector Machine

Hypothesis class: $\mathcal{H} = \{h_w(x) = w^\top x : w \in \mathbb{R}^d\}$

Loss: $\ell_{\text{hinge}}(m) = \max(1 - m, 0)$ (hinge loss)

Regularizer: ℓ_2

Empirical risk minimization:

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \max(1 - y^{(i)} h_w(x^{(i)}), 0) + \lambda \|w\|_2^2$$

Classification Losses

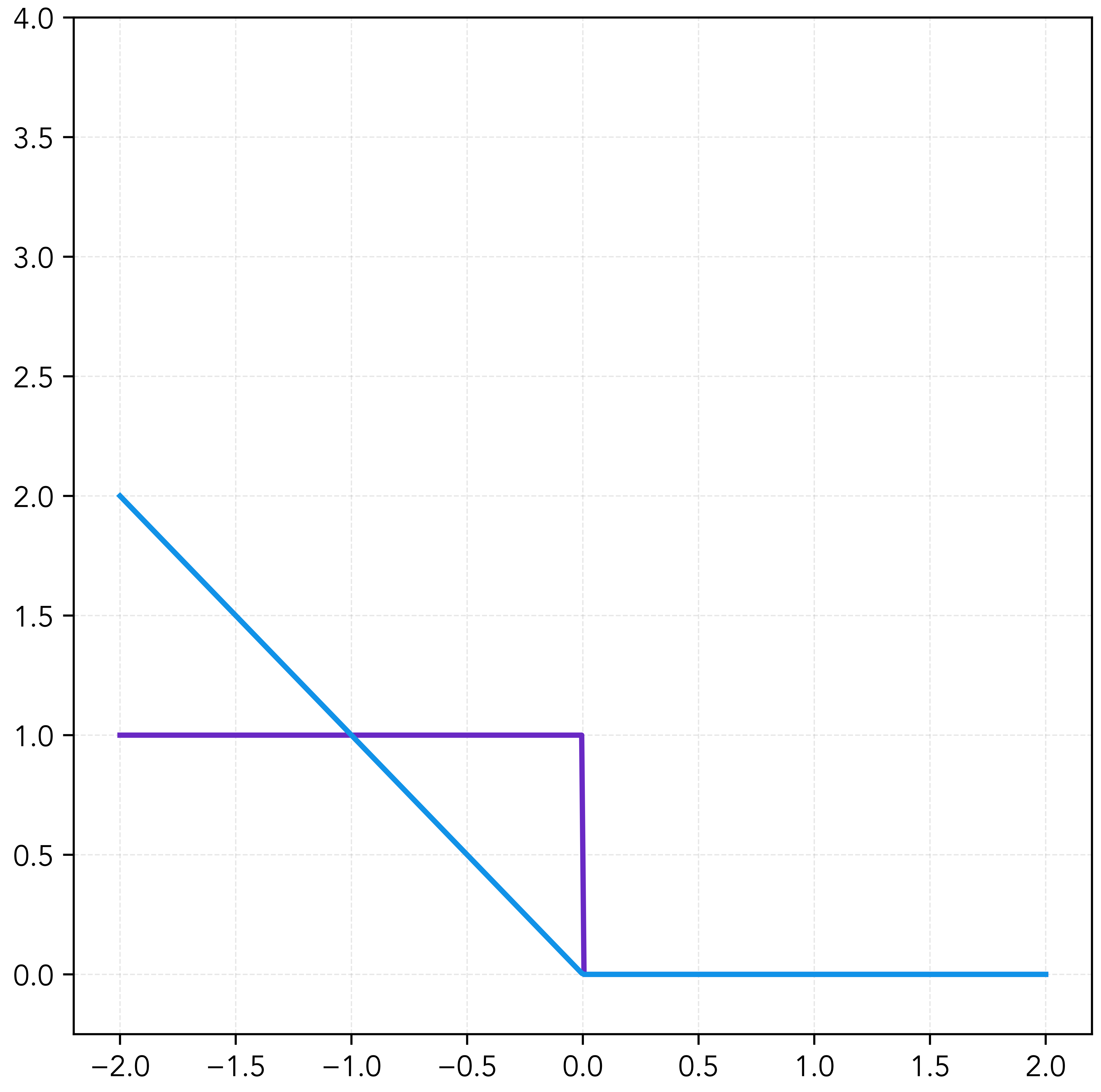
Perceptron Loss

Margin: $m = \hat{y}y$

Perceptron loss: $\ell_{\text{perc}}(m) := \max(-m, 0)$

Hinge loss, with "hinge at zero."

Not an upper bound on zero-one loss, but it is **convex**.



Perceptron Loss

Perceptron Algorithm

Hypothesis class: $\mathcal{H} = \{h_w(x) = w^\top x : w \in \mathbb{R}^d\}$

"SGD" on the perceptron loss $\ell_{\text{perc}}(m) = \max(-m, 0)$ (perceptron loss) is equivalent to:

```
Initialize $w \leftarrow 0$.
While there exists $(x^{(i)}, y^{(i)})$ that is misclassified:
    For $(x^{(i)}, y^{(i)}) \in D_n$:
        If $y^{(i)} w^\top x^{(i)} < 0$ (wrong prediction):
            Update $w \leftarrow w + y^{(i)} x^{(i)}$.
```

Classification Losses

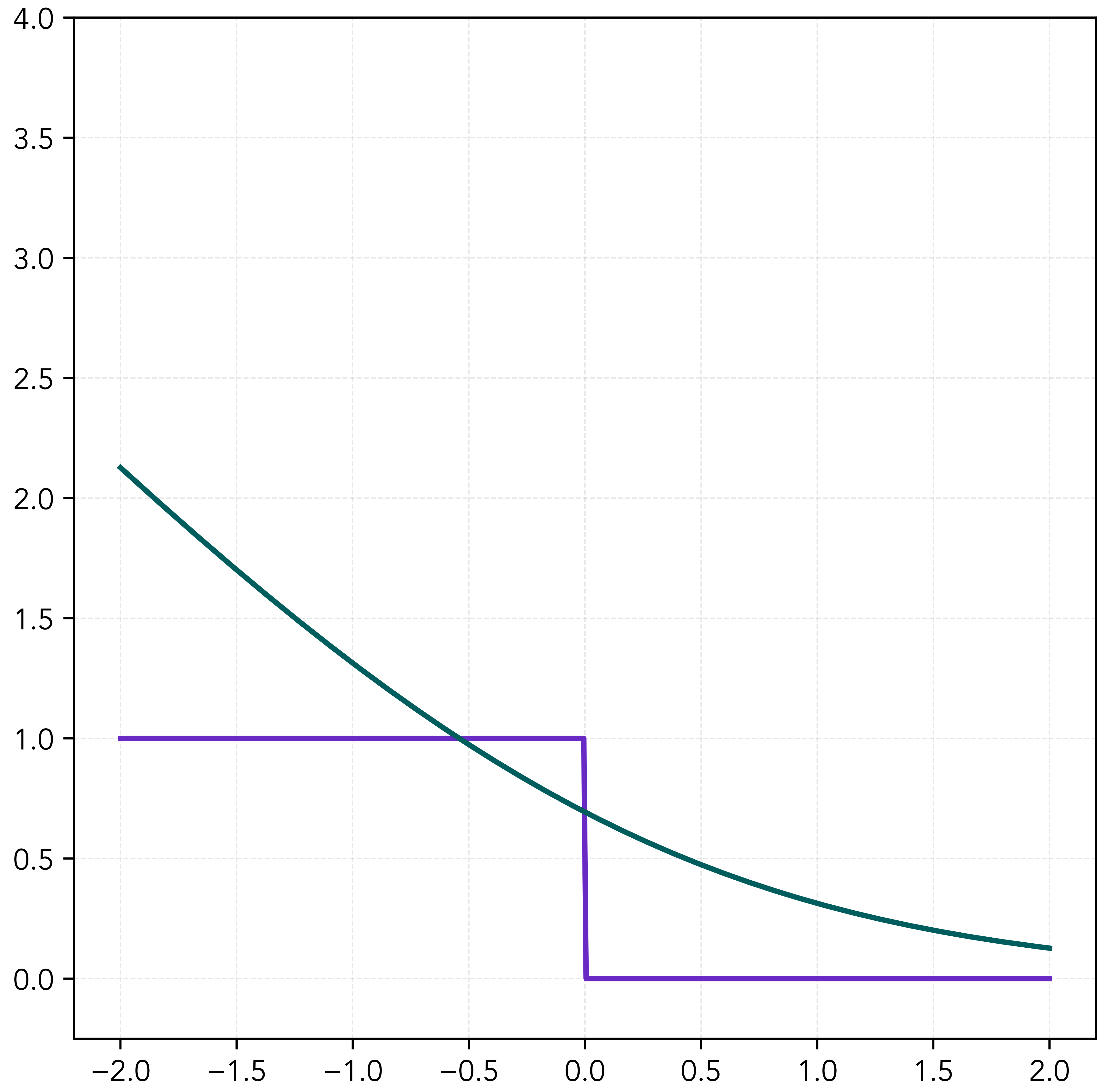
Logistic Loss

Margin: $m = \hat{y}y$

Logistic/Log loss: $\ell_{\log}(m) := \log(1 + e^{-m})$

Logistic loss is **differentiable**.

Always rewards more margin (loss never 0).



Logistic Loss

Logistic Regression

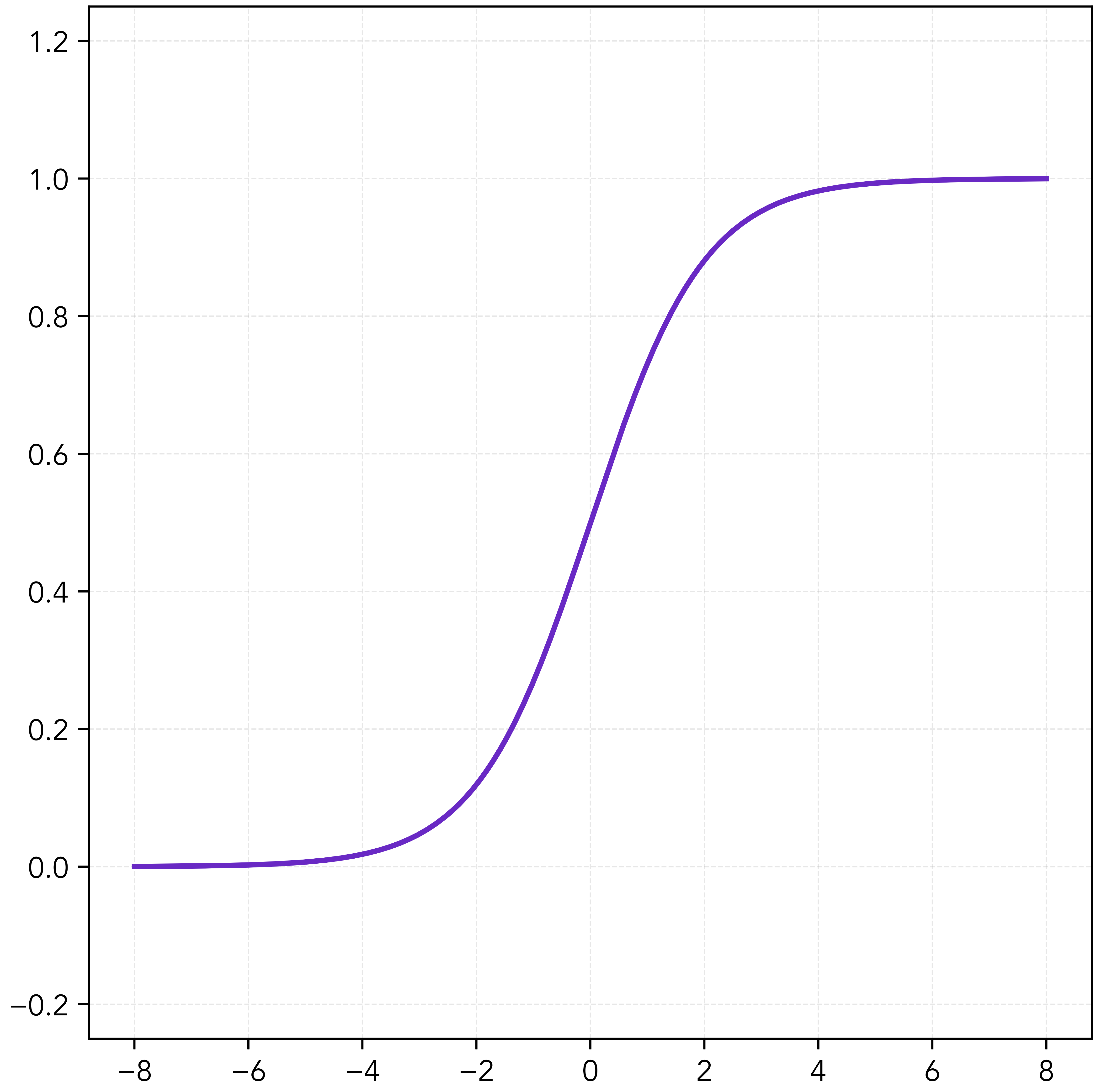
Suppose we want some $h : \mathbb{R}^d \to [0,1]$ (to be interpreted as *probability* of -1 or 1).

The sigmoid function $\phi : \mathbb{R} \to [0,1]$:

$$\phi(z) := \frac{1}{1 + \exp(-z)}$$

Useful property:

$$1 - \phi(z) = \phi(-z).$$



Logistic Loss

Logistic Regression

$$\phi(z) := \frac{1}{1+\exp(-z)}$$

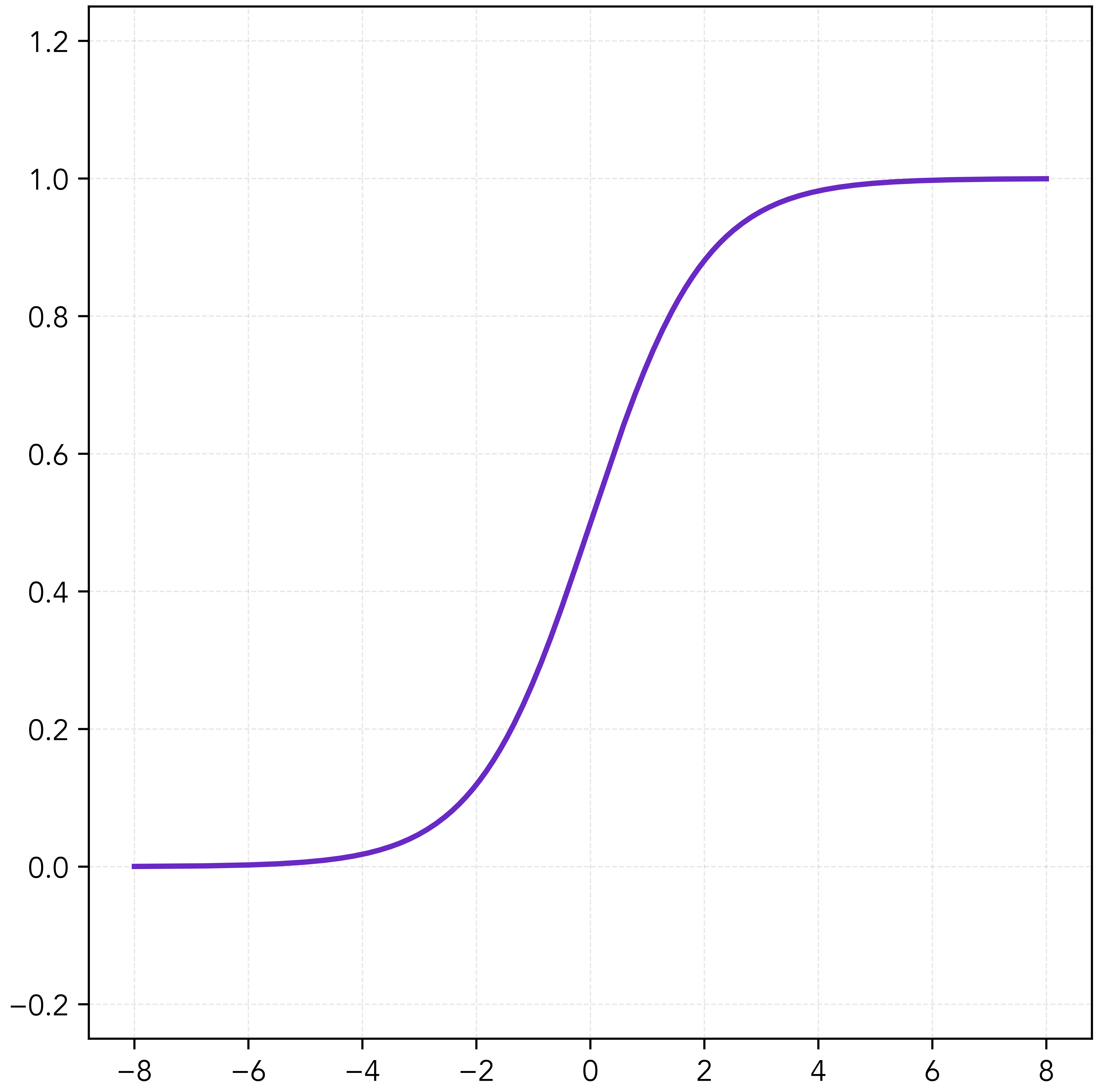
Compose sigmoid with linear functions:

$$\mathcal{F}_{\text{sig}} := \{x \mapsto \phi(w^\top x) : w \in \mathbb{R}^d\}$$

If $w^\top x \gg 0$, $\phi(w^\top x)$ is close to 1.

If $w^\top x \ll 0$, $\phi(w^\top x)$ is close to 0.

If $w^\top x \approx 0$, $\phi(w^\top x)$ is close to $1/2$.



Logistic Loss

Logistic Regression

$$\phi(z) := \frac{1}{1+\exp(-z)} \text{ and hypothesis class } \mathcal{F}_{\text{sig}} := \{x \mapsto \phi(w^\top x) : w \in \mathbb{R}^d\}$$

What's a reasonable loss function?

If $y = 1$, we want $\phi(w^\top x)$ large (probability of predicting 1).

If $y = -1$, we want $\phi(w^\top x)$ small (probability of predicting -1) $\Longrightarrow 1 - \phi(w^\top x)$ large.

Important property of sigmoid: $1 - \phi(z) = \phi(-z)$.

If $y = -1$, we want $1 - \phi(w^\top x) = \phi(-w^\top x)$ large.

Logistic Loss

Logistic Regression

What's a reasonable loss function?

If $y = 1$, we want $\phi(w^\top x)$ large (probability of predicting 1).

If $y = -1$, we want $\phi(-w^\top x)$ large (probability of predicting -1).

Summary. For $y \in \{-1,1\}$, we want $\phi(yw^\top x)$ large $\implies$ Smaller loss for larger $\phi(yw^\top x)$.

$$-\log(\phi(yw^\top x)) = -\log\left(\frac{1}{1+\exp(-yw^\top x)}\right) = \log(1+\exp(-yw^\top x))$$

Classification Losses

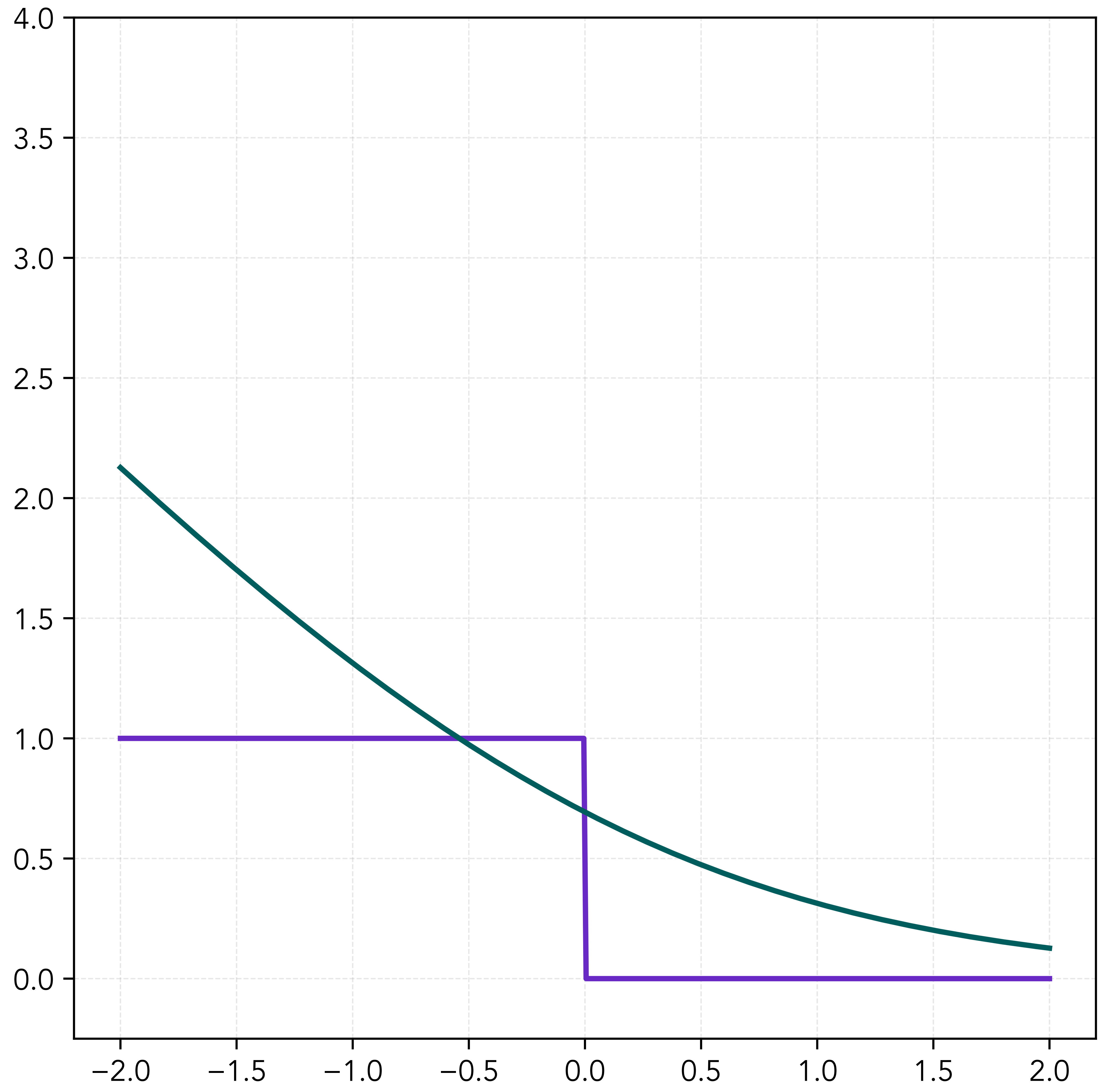
Logistic Loss

Margin: $m = \hat{y}y$

Logistic/Log loss: $\ell_{\log}(m) := \log(1 + e^{-m})$

Logistic loss is **differentiable**.

Always rewards more margin (loss never 0).



Logistic Loss

Logistic Regression

Hypothesis class: $\mathcal{H} = \{h_w(x) = w^\top x : w \in \mathbb{R}^d\}$

Loss: $\ell_{\log}(m) := \log(1 + e^{-m})$ (logistic loss)

Empirical risk minimization:

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y^{(i)} w^\top x^{(i)}))$$

Minimizing this objective is known as logistic regression (a linear **classification** method).

Square Loss

Square loss for classification?

Recall the square loss: $\ell(f(x), y) = (f(x) - y)^2$.

For $y \in \{-1, 1\}$, we have $y^2 = 1$, so we can write this in terms of the margin:

$$\ell(f(x), y) = (f(x) - y)^2 = f^2(x)y^2 - 2f(x)y + 1 = (1 - f(x)y)^2 = (1 - m)^2$$

Classification Losses

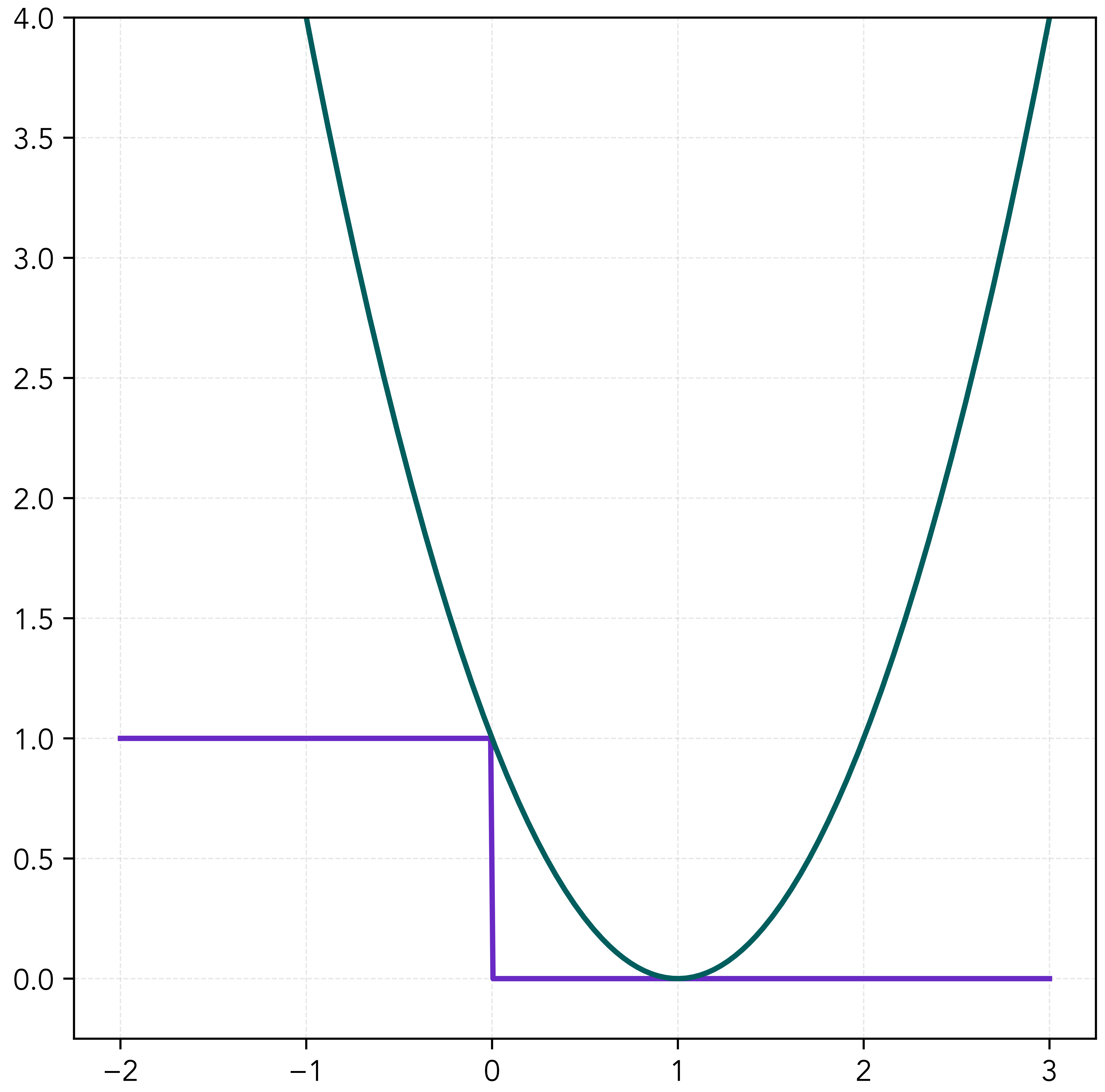
Square Loss

Margin: $m = \hat{y}y$

Square loss: $\ell_{\text{square}}(m) := (1 - m)^2$

Convex and differentiable.

Heavily penalizes outliers (e.g. mislabeled examples).



Classification Losses

Convexity

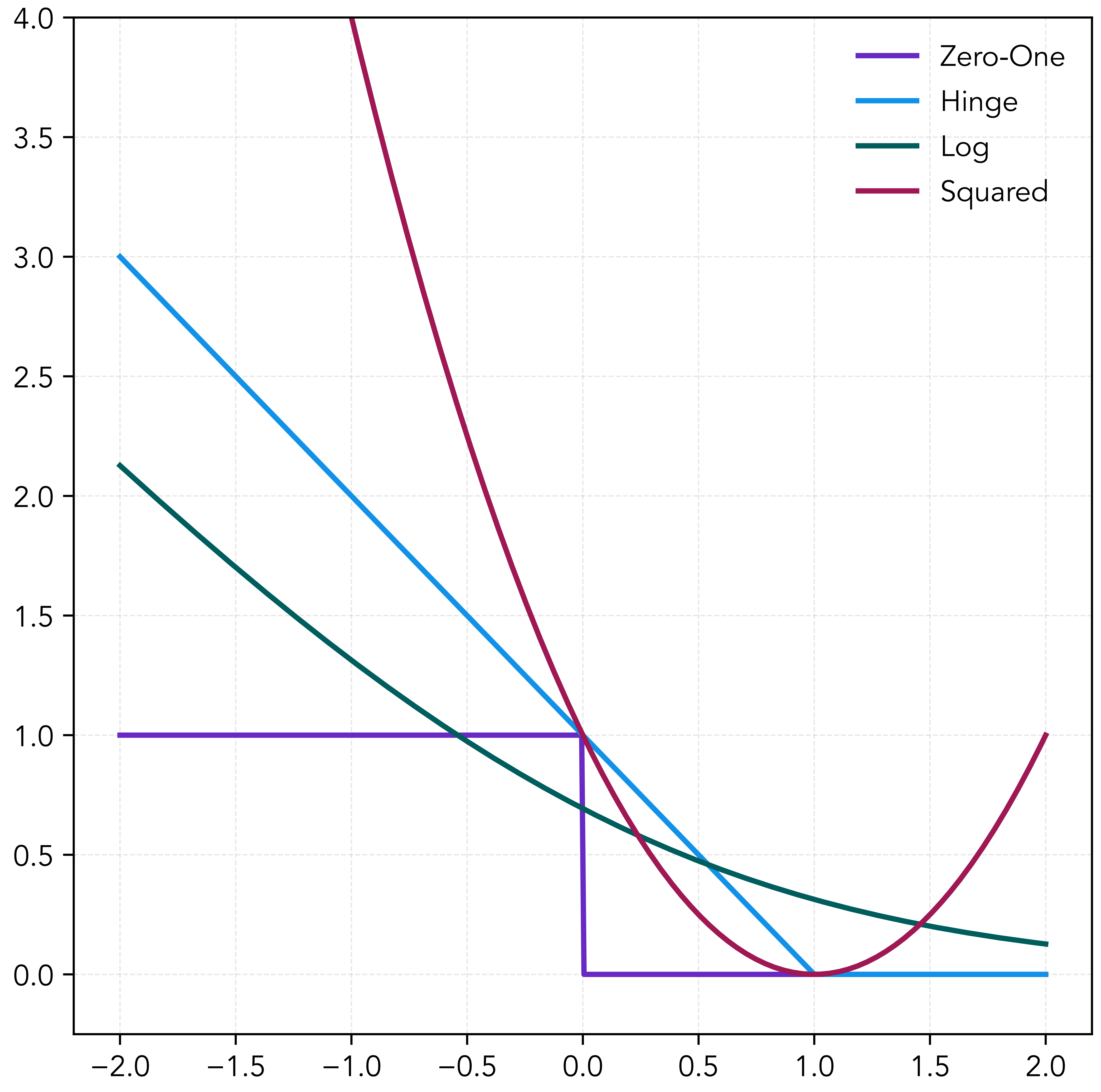
All of these losses have a property in common: **convexity**.

$$\ell_{\text{hinge}}(m) := \max(1 - m, 0)$$

$$\ell_{\text{perc}}(m) := \max(-m, 0)$$

$$\ell_{\log}(m) := \log(1 + e^{-m})$$

$$\ell_{\text{square}}(m) := (1 - m)^2$$



Outline