

# 10-301/601: Introduction to Machine Learning

## Lecture 10 – Regularization

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19/2/23

# Recall: Logistic Regression

- Model:  
$$p(y|x, \theta) = \begin{cases} \sigma(\theta^T x) & \text{if } y = 1 \\ 1 - \sigma(\theta^T x) & \text{if } y = 0 \end{cases}$$
 where  $\sigma(z) = 1/(1 + \exp(-z))$
- Derivatives
$$\frac{\partial J^{(i)}}{\partial \theta_m} = \frac{\partial}{\partial \theta_m} (-\log p(y^{(i)}|x^{(i)}, \theta)) \\ = -\left(y^{(i)} - \sigma(\theta^T x^{(i)})\right)x_m^{(i)}$$
- Optimization: use GD or SGD;  
logistic regression does not permit a closed form solution

- Objective: minimize the negative conditional log-likelihood

$$J(\theta) = \frac{1}{N} \sum_{i=1}^N -\log p(y^{(i)}|x^{(i)}, \theta)$$

- Gradients

$$\nabla J^{(i)}(\theta) = -\left(y^{(i)} - \sigma(\theta^T x^{(i)})\right)x^{(i)}$$

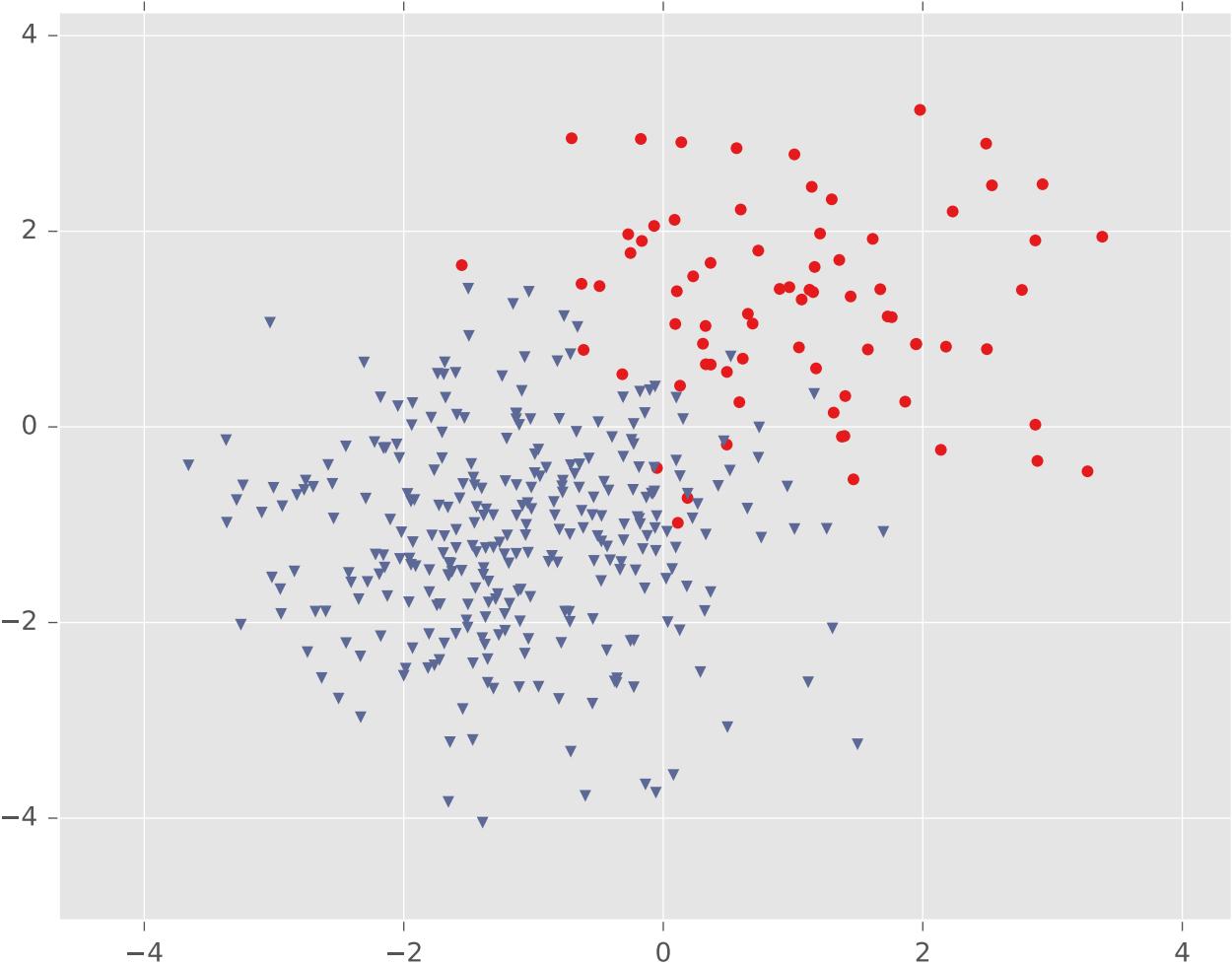
$$\nabla J(\theta) = \frac{1}{N} \sum_{i=1}^N \nabla J^{(i)}$$

- Predictions

$$\hat{y} = \underset{y \in \{0,1\}}{\operatorname{argmax}} p(y|x', \hat{\theta})$$

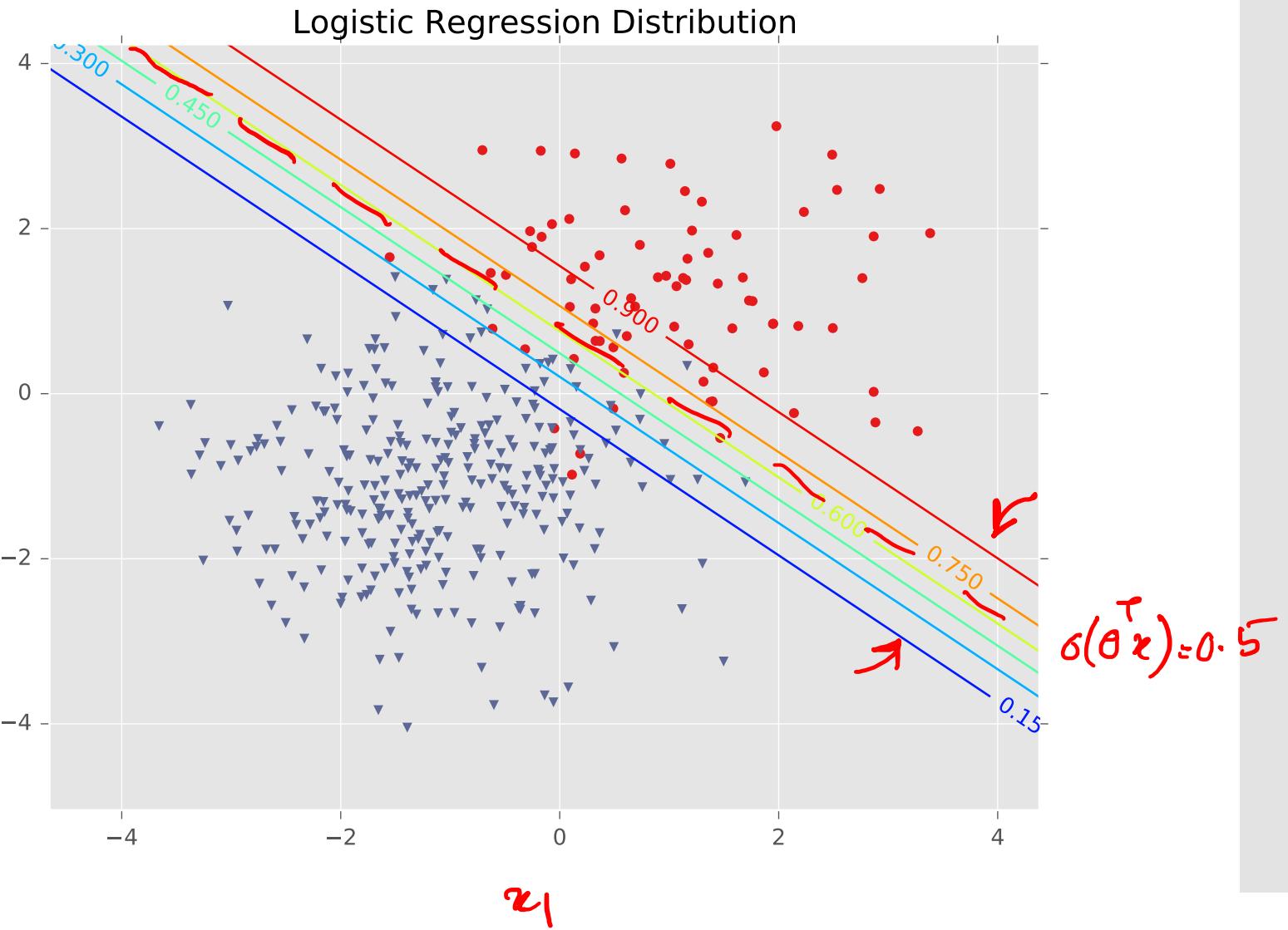
$$= \text{"sign"}(\hat{\theta}^T x')$$

# Logistic Regression Decision Boundary

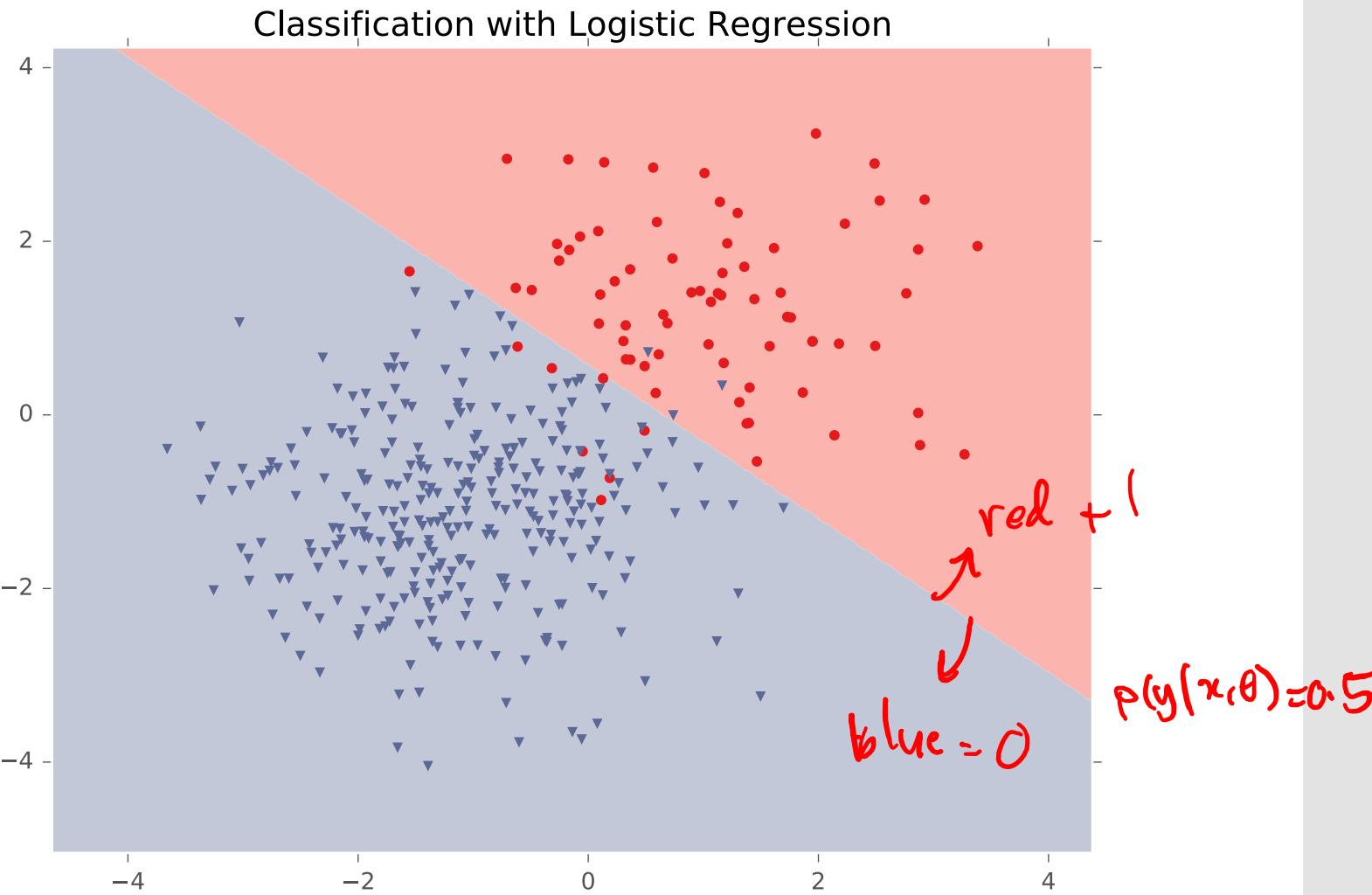


# Logistic Regression Decision Boundary

$\chi_2$

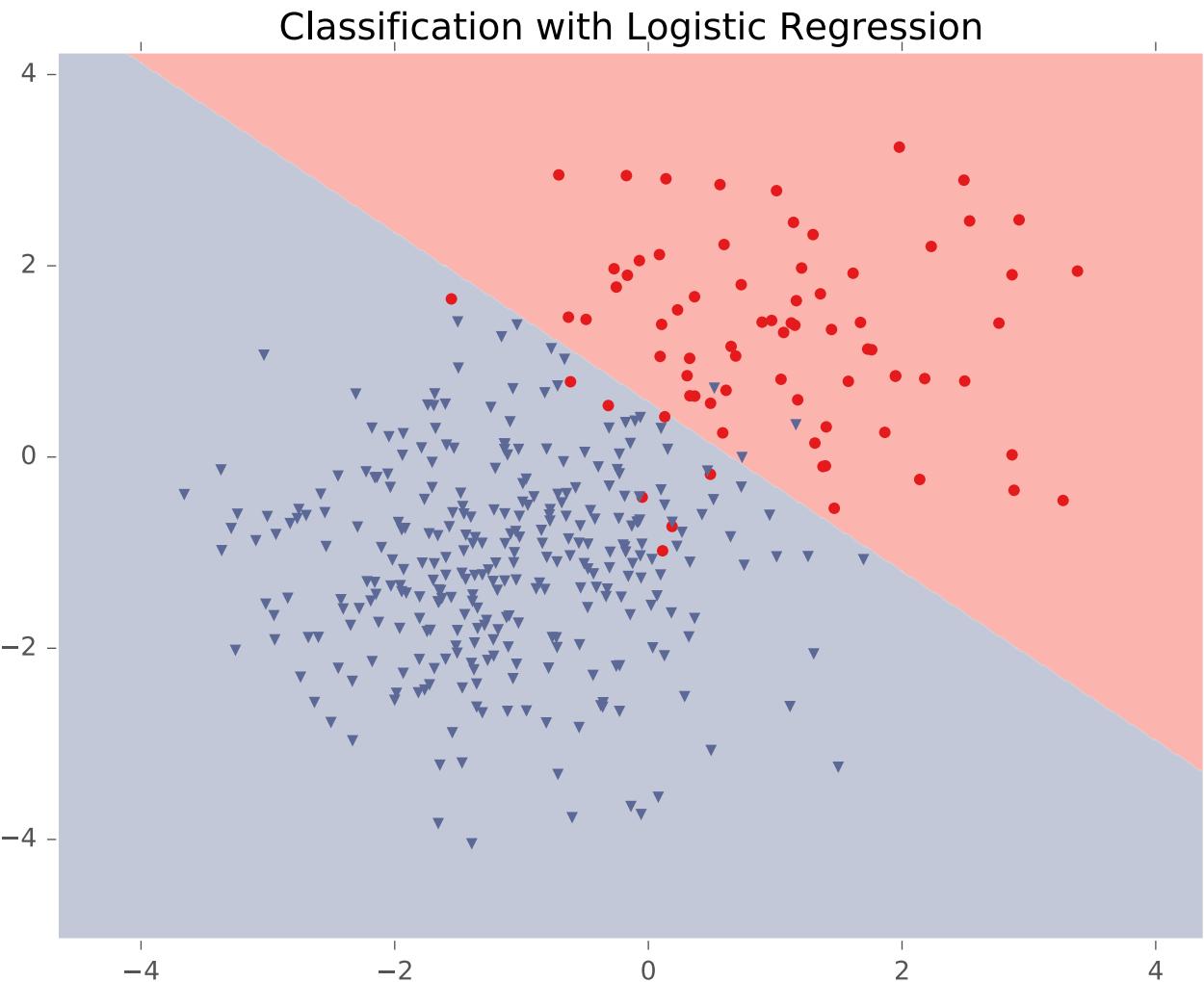


# Logistic Regression Decision Boundary



But is this the  
best that we  
could do, even  
if we knew  $p^*$ ?

$$p(y=1 | x, \theta) = p^*(y=1 | x)$$



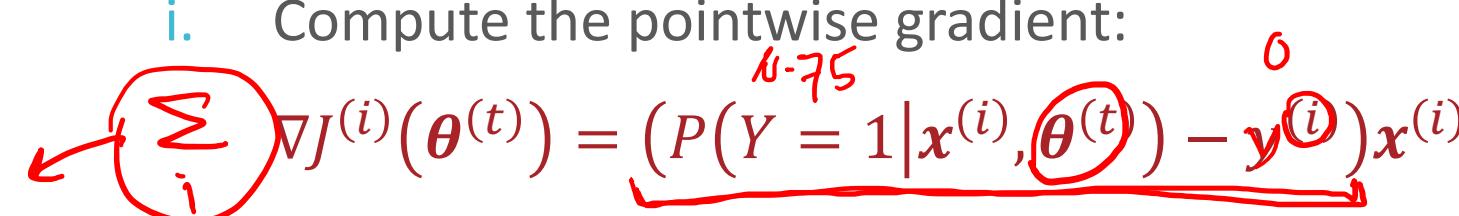
# Bayes Optimal Classifier

- Suppose you knew  $p^*(Y = 1|x)$  for all  $x$  and wanted to minimize the 0-1 loss
$$\rightarrow \ell(\hat{y}, y) = \mathbb{1}(\hat{y} \neq y)$$
$$p^*(y=1|x) = 0.75$$
  - Then the optimal classifier in this setting, called the *Bayes optimal classifier*, is
- $$\hat{y} = \begin{cases} 1 & \text{if } p^*(Y = 1|x) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$
- Exercise.*
- 
- The graph illustrates the Bayes optimal classifier decision boundary. The x-axis represents the input feature  $x$ , and the y-axis represents the probability density functions  $p(y=1|x)$  and  $p(y=0|x)$ . The blue curve represents  $p(y=0|x)$  and the red curve represents  $p(y=1|x)$ . The two curves intersect at a point  $x$  on the x-axis. For  $x <$  this intersection point,  $p(y=0|x) > p(y=1|x)$ , so the classifier outputs 0. For  $x >$  this intersection point,  $p(y=1|x) > p(y=0|x)$ , so the classifier outputs 1. The intersection point is the decision boundary where the classifier outputs 0.5. Handwritten annotations include  $p(y=1|x)$  above the red curve and  $p(y=0|x, \theta)$  above the blue curve.
- The *reducible error* of a classifier is the expected loss that could be eliminated if we knew  $p^*$
  - The *irreducible error* of a classifier is the expected loss even if we knew  $p^*$

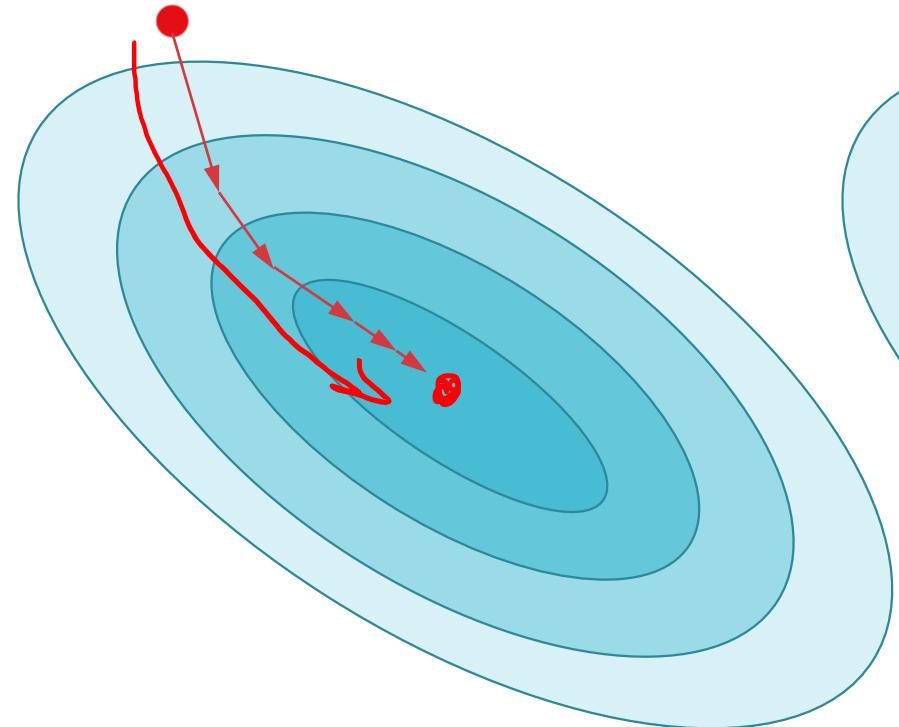
# Stochastic Gradient Descent (SGD) for Logistic Regression

- Input: training dataset  $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$  and step size  $\gamma$
- 1. Initialize  $\theta^{(0)}$  to all zeros and set  $t = 0$
- 2. While TERMINATION CRITERION is not satisfied
  - a. For  $i \in \text{shuffle}(\{1, \dots, N\})$ 
    - i. Compute the pointwise gradient:
$$\nabla J^{(i)}(\theta^{(t)}) = - (y^{(i)} - \sigma(\theta^T x^{(i)})) x^{(i)}$$
    - ii. Update  $\theta$ :  $\theta^{(t+1)} \leftarrow \theta^{(t)} - \gamma \nabla J^{(i)}(\theta^{(t)})$
    - iii. Increment  $t$ :  $t \leftarrow t + 1$
  - Output:  $\theta^{(t)}$

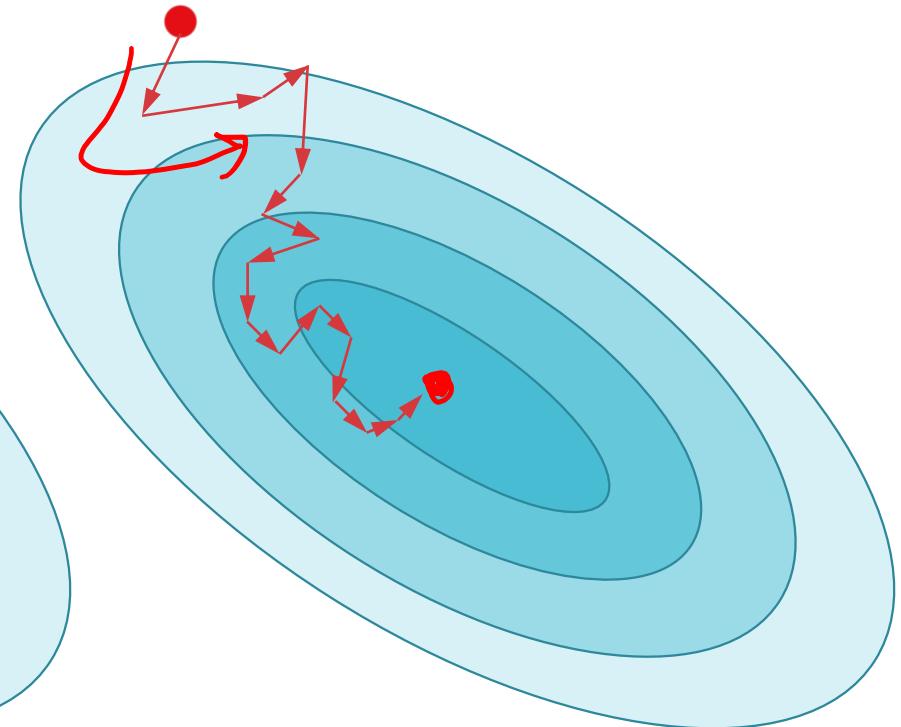
# Stochastic Gradient Descent (SGD) for Logistic Regression

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    - i. Compute the pointwise gradient:  
$$\nabla J^{(i)}(\theta^{(t)}) = \left( P(Y=1|x^{(i)}, \theta^{(t)}) - y^{(i)} \right) x^{(i)}$$

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# Stochastic Gradient Descent vs. Gradient Descent

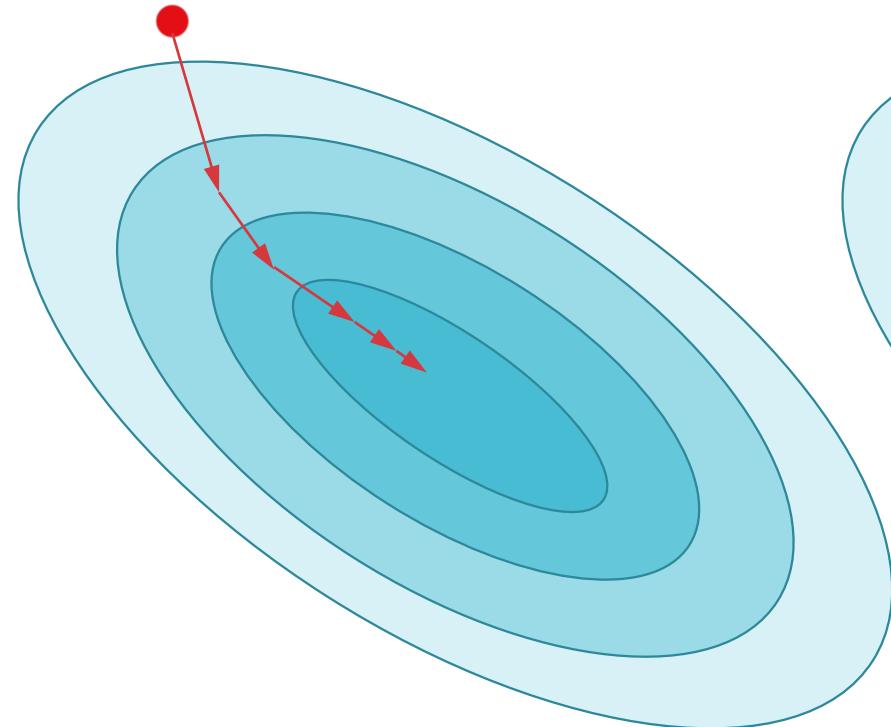


Gradient Descent

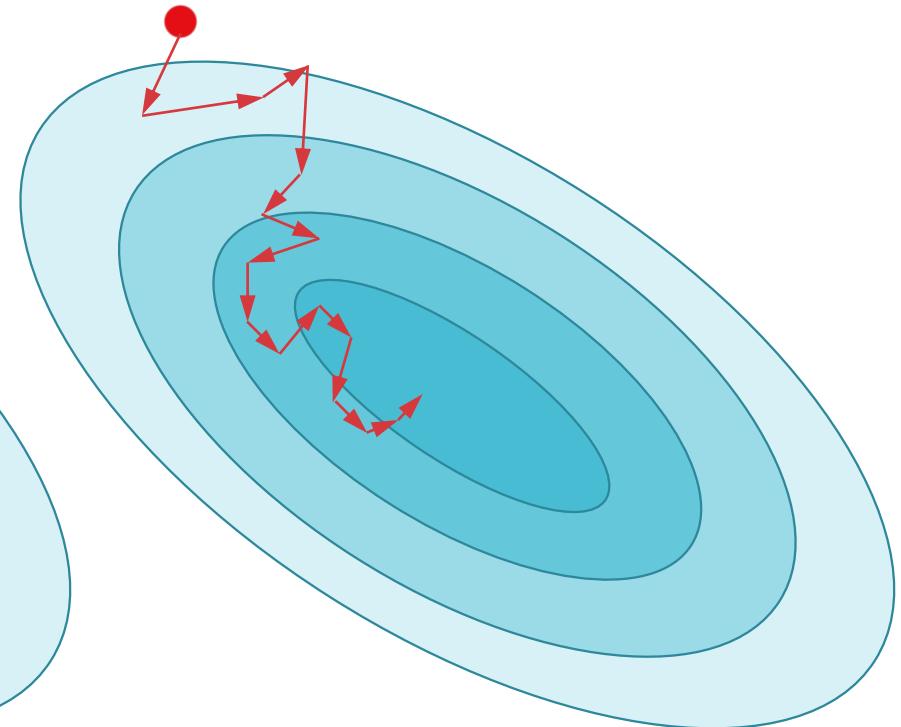


Stochastic Gradient Descent

Can we find  
some middle  
ground here?



Gradient Descent



Stochastic Gradient Descent

# Mini-batch Stochastic Gradient Descent for Neural Networks

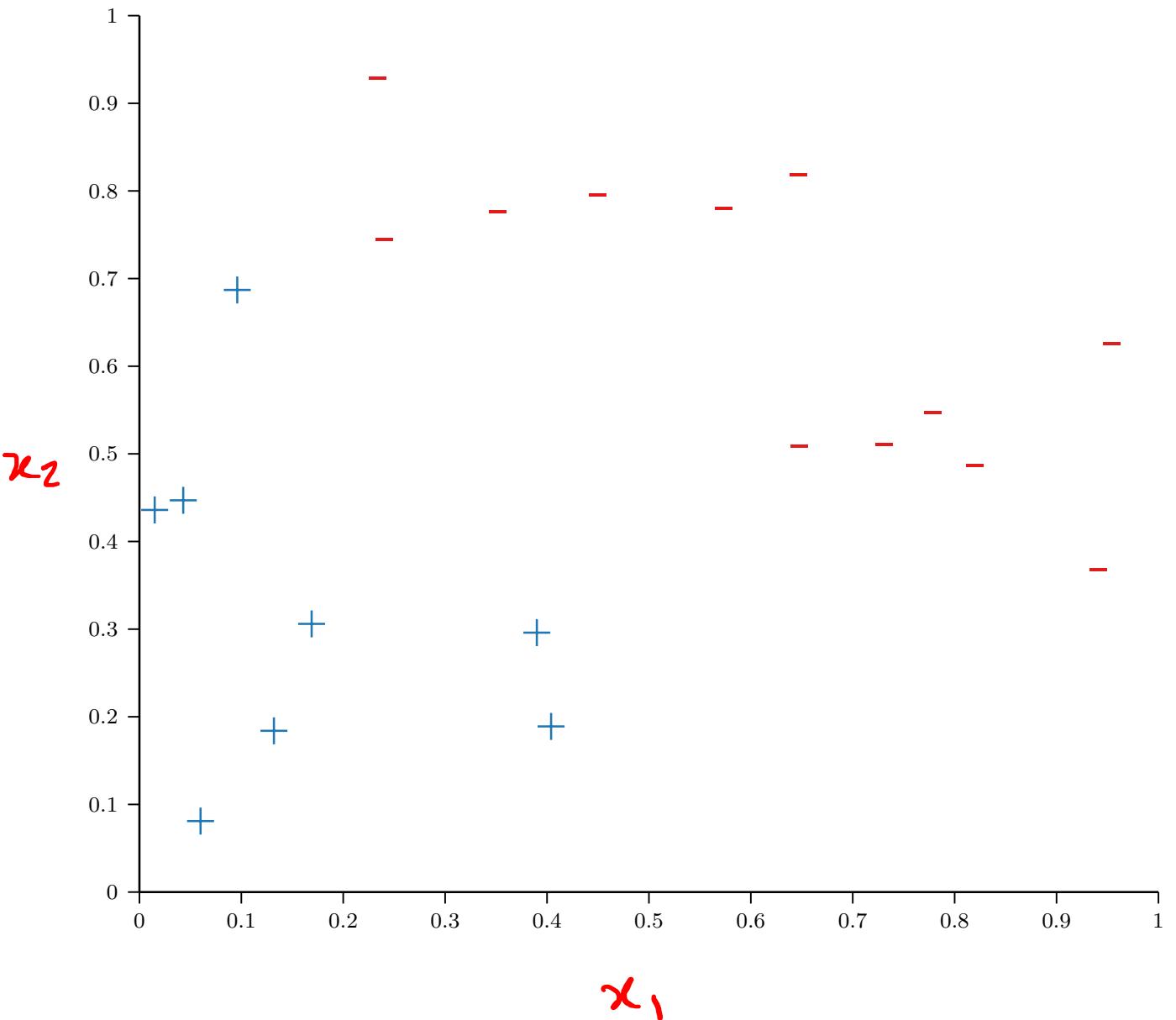
- Input: training dataset  $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , step size  $\gamma$ , and batch size  $B$
- 1. Initialize  $\boldsymbol{\theta}^{(0)}$  to all zeros and set  $t = 0$
- 2. While TERMINATION CRITERION is not satisfied
  - a. Randomly sample  $B$  data points from  $\mathcal{D}$ ,  $\{(\mathbf{x}^{(b)}, y^{(b)})\}_{b=1}^B$
  - b. Compute the gradient w.r.t. the sampled *batch*,  
$$\nabla J^{(B)}(\boldsymbol{\theta}^{(t)}) = \frac{1}{B} \sum_{b=1}^B (P(Y = 1 | \mathbf{x}^{(b)}, \boldsymbol{\theta}^{(t)}) - y^{(b)}) \mathbf{x}^{(b)}$$
  - c. Update  $\boldsymbol{\theta}$ :  $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla J^{(B)}(\boldsymbol{\theta}^{(t)})$
  - d. Increment  $t$ :  $t \leftarrow t + 1$
- Output:  $\boldsymbol{\theta}^{(t)}$

# Logistic Regression Learning Objectives

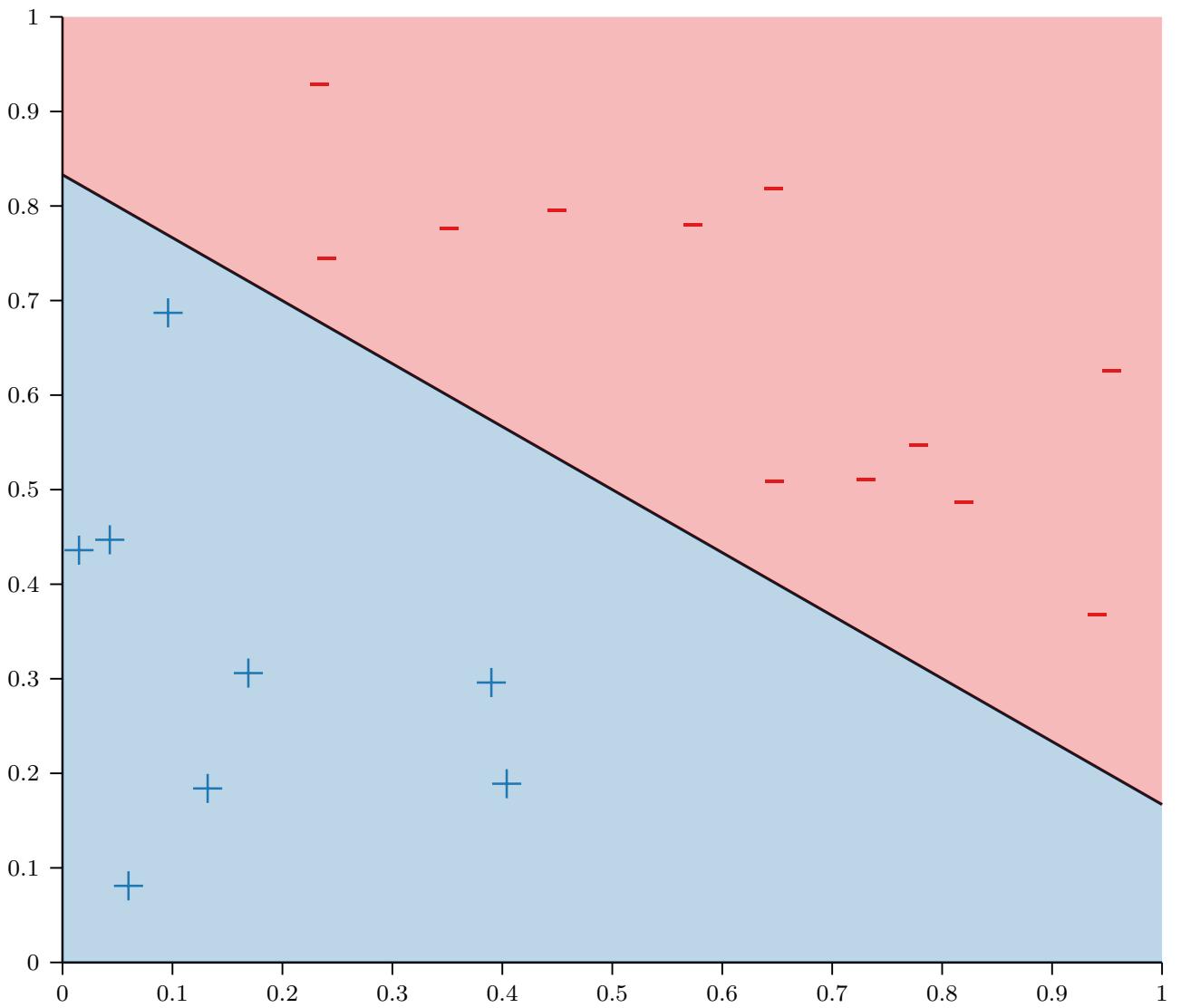
You should be able to...

- Apply the principle of maximum likelihood estimation (MLE) to learn the parameters of a probabilistic model
- Given a discriminative probabilistic model, derive the conditional log-likelihood, its gradient, and the corresponding Bayes Classifier
- Explain the practical reasons why we work with the log of the likelihood
- Implement logistic regression for binary classification
- Prove that the decision boundary of binary logistic regression is linear

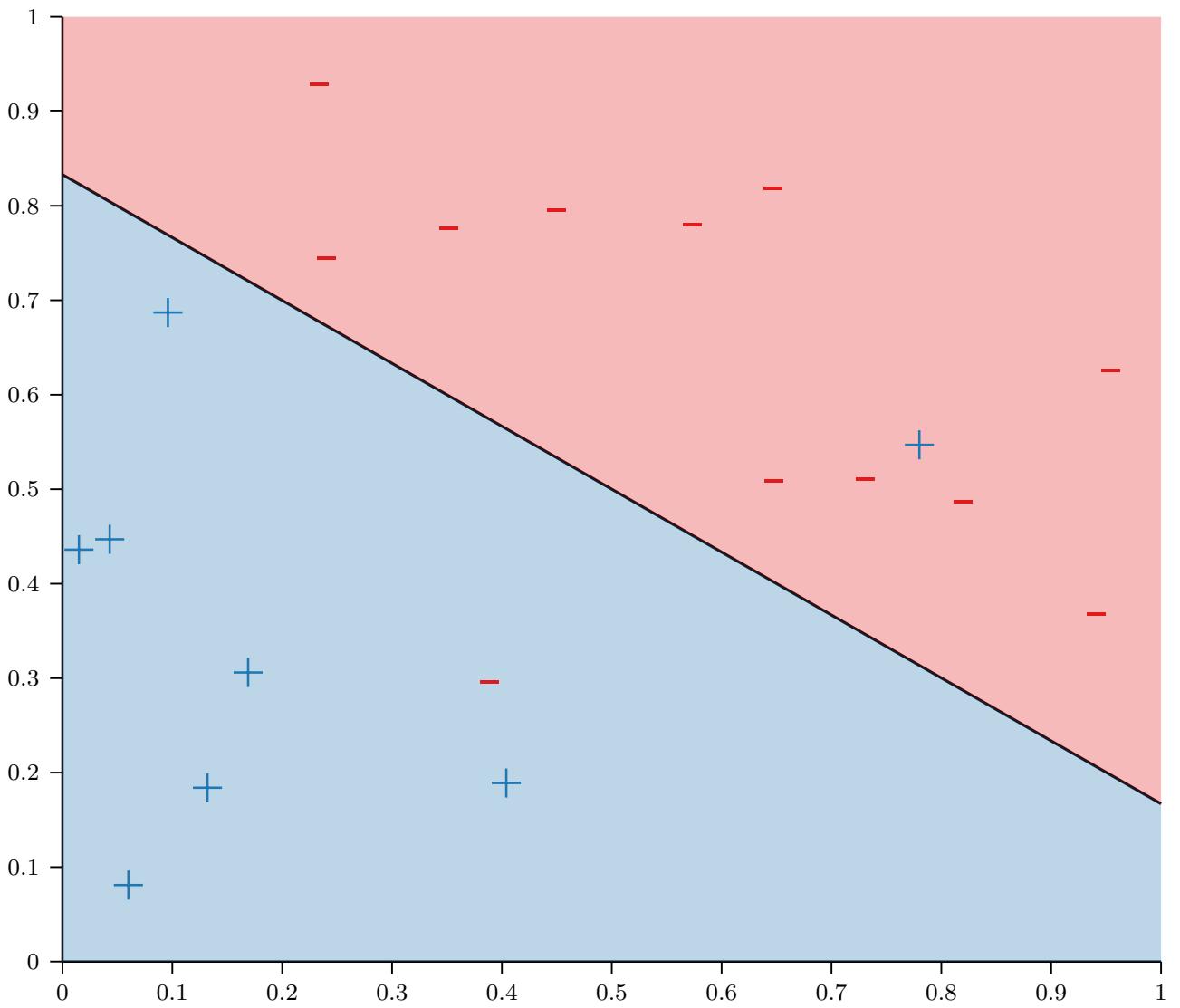
# Linear Models



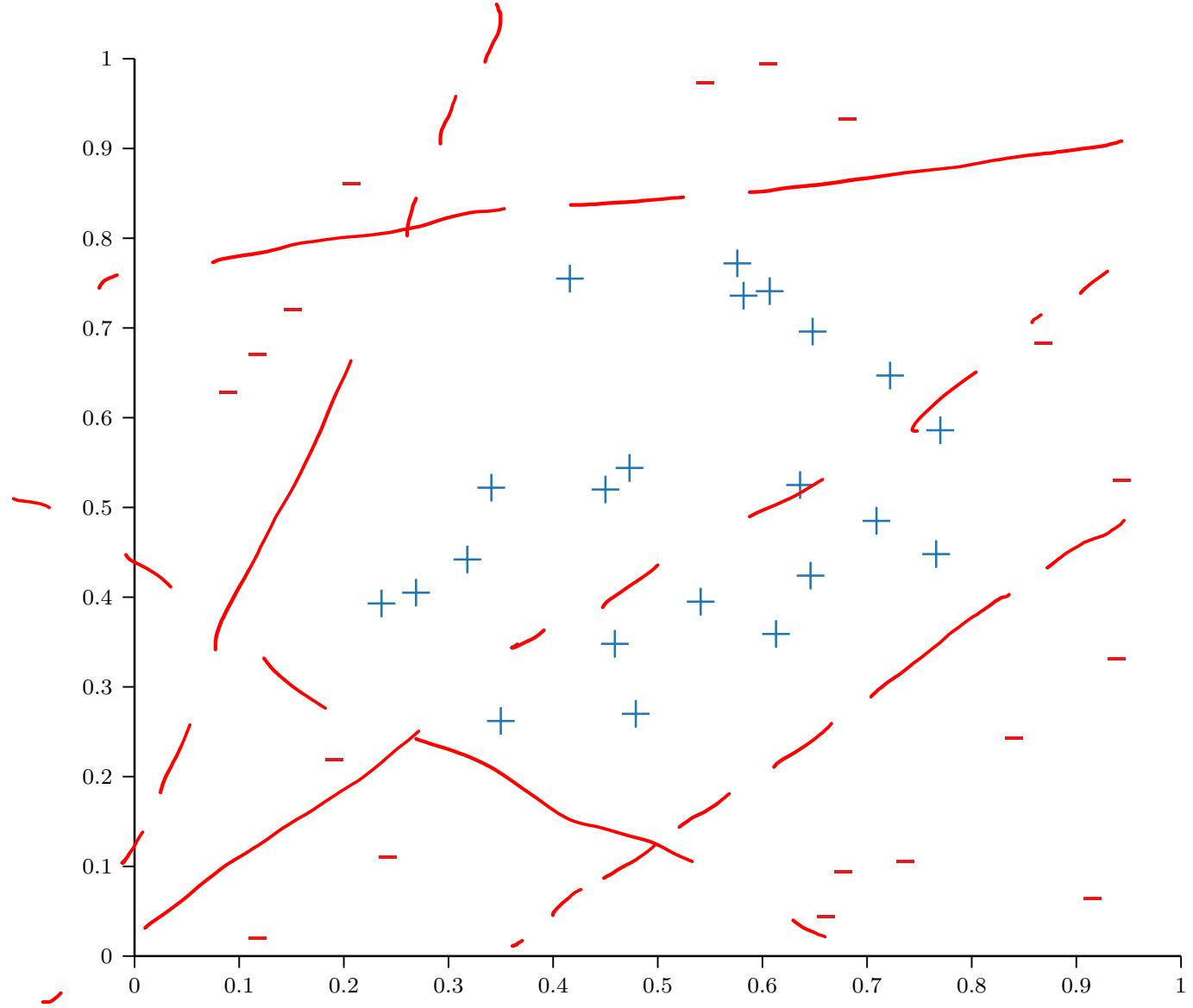
# Linear Models



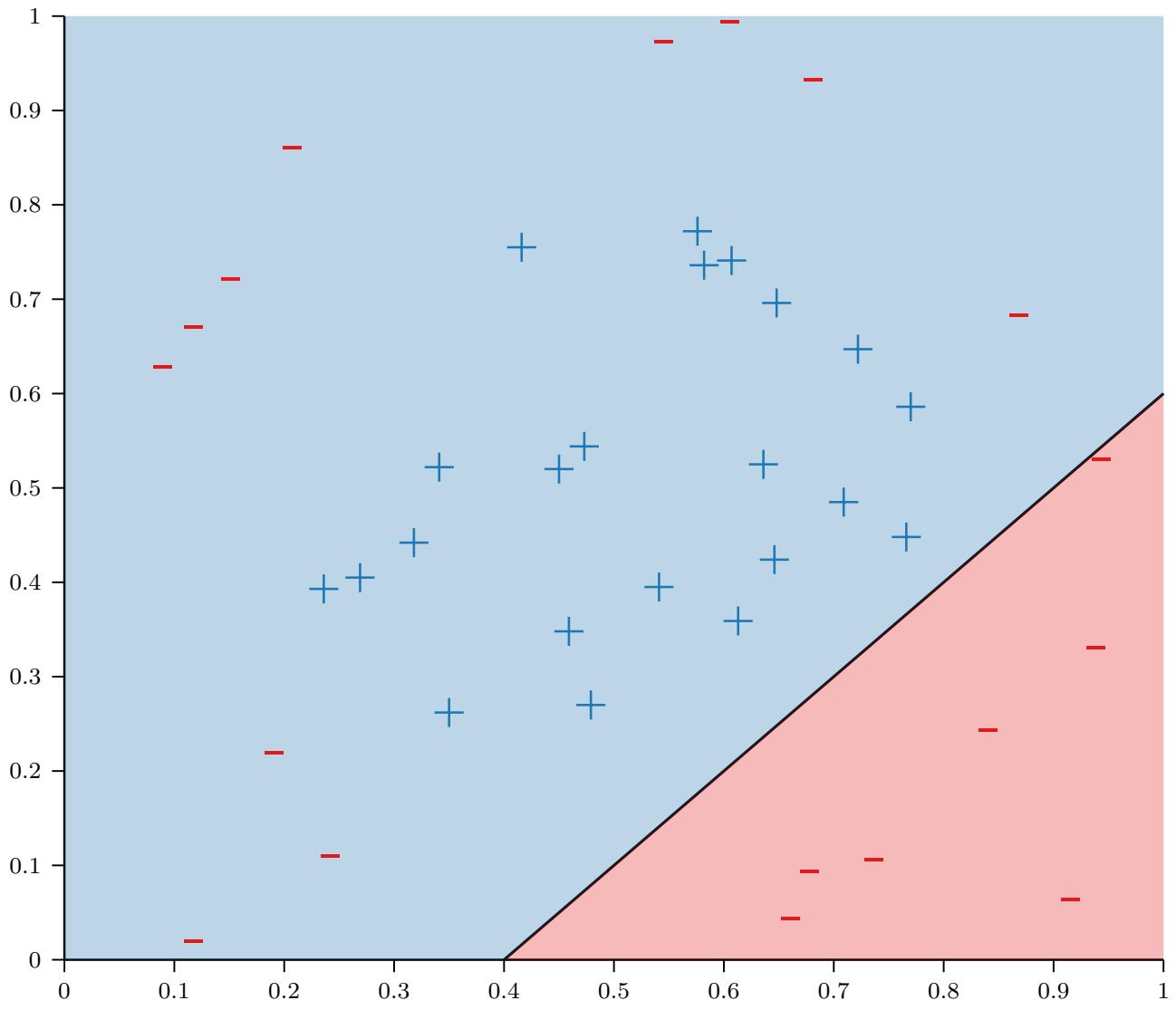
# Linear Models



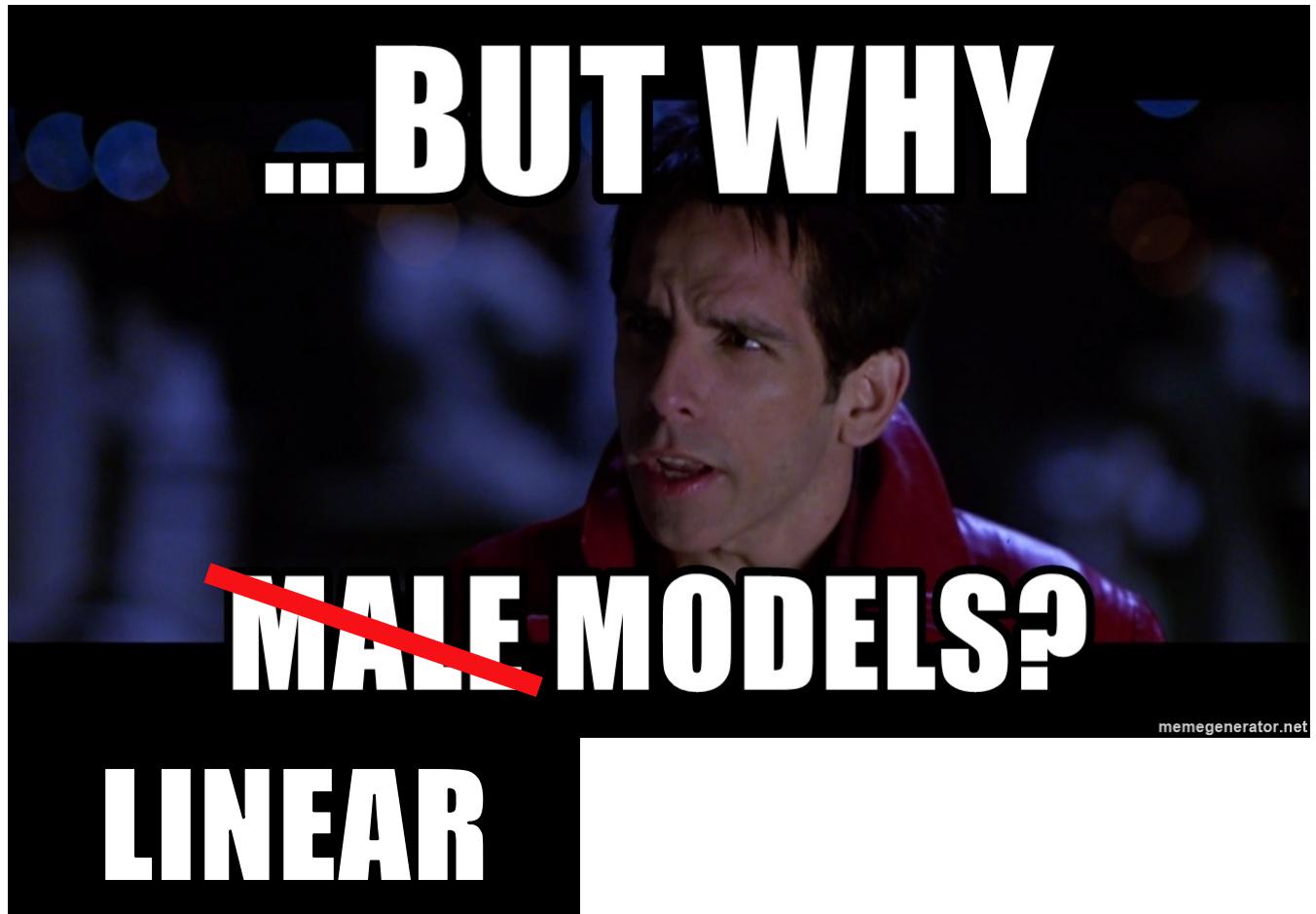
# Linear Models?



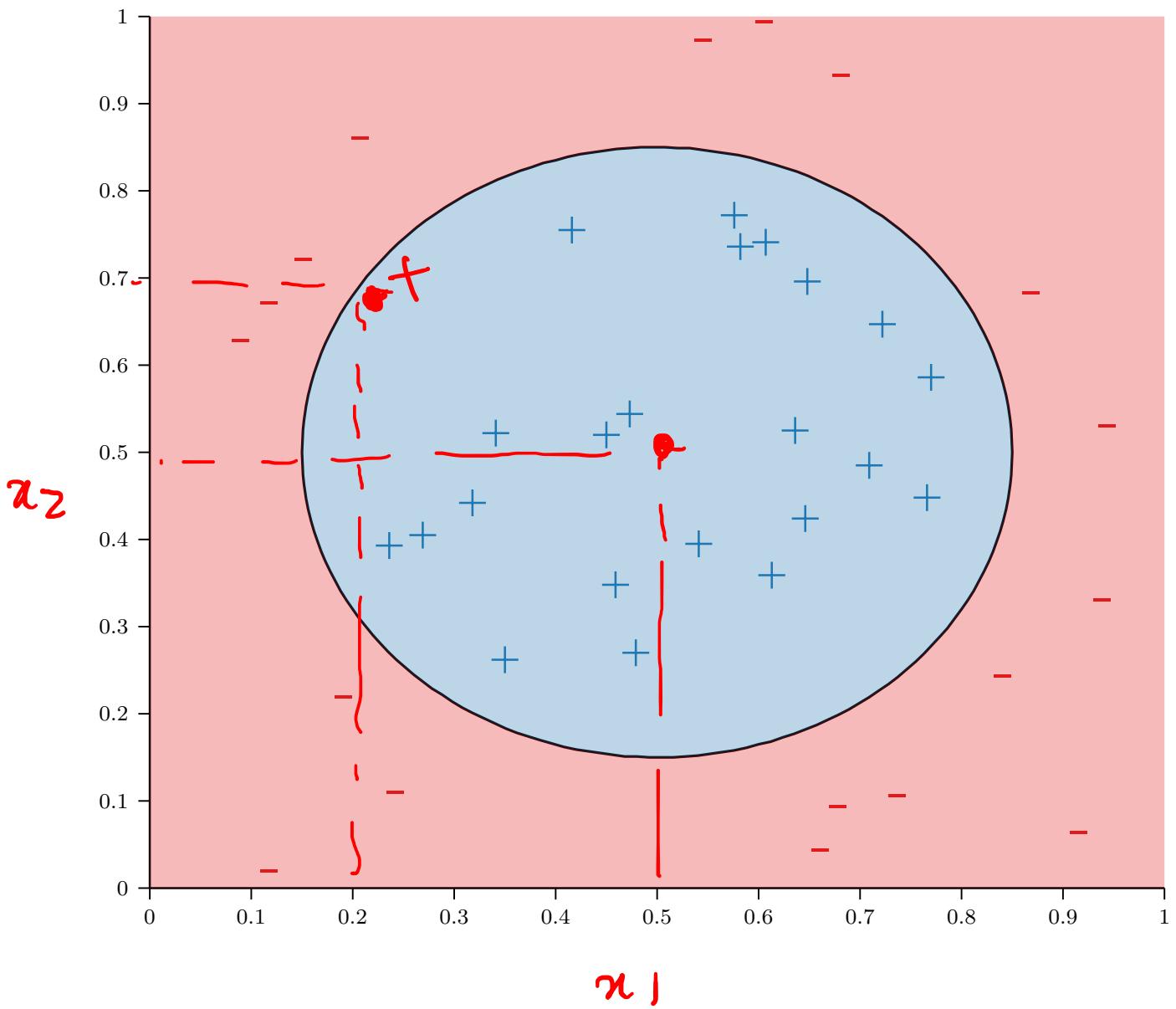
# Linear Models?



# Linear Models?



# Nonlinear Models



# Feature Transforms

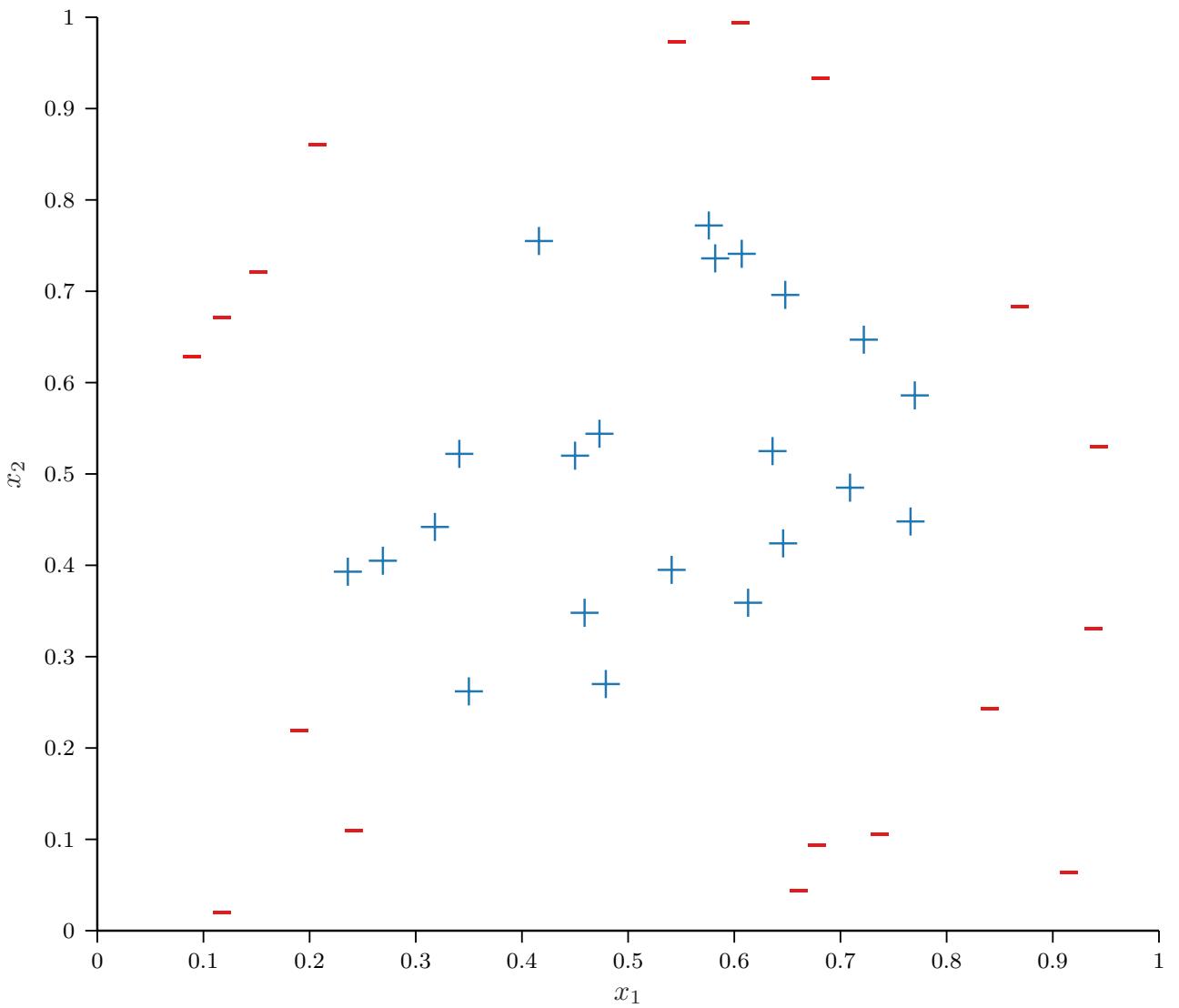
- Given  $D$ -dimensional inputs  $\mathbf{x} = [x_1, \dots, x_D]$ , first compute some transformation of our input, e.g.,

$$\phi([x_1, x_2]) = [z_1 = (x_1 - 0.5)^2, z_2 = (x_2 - 0.5)^2]$$

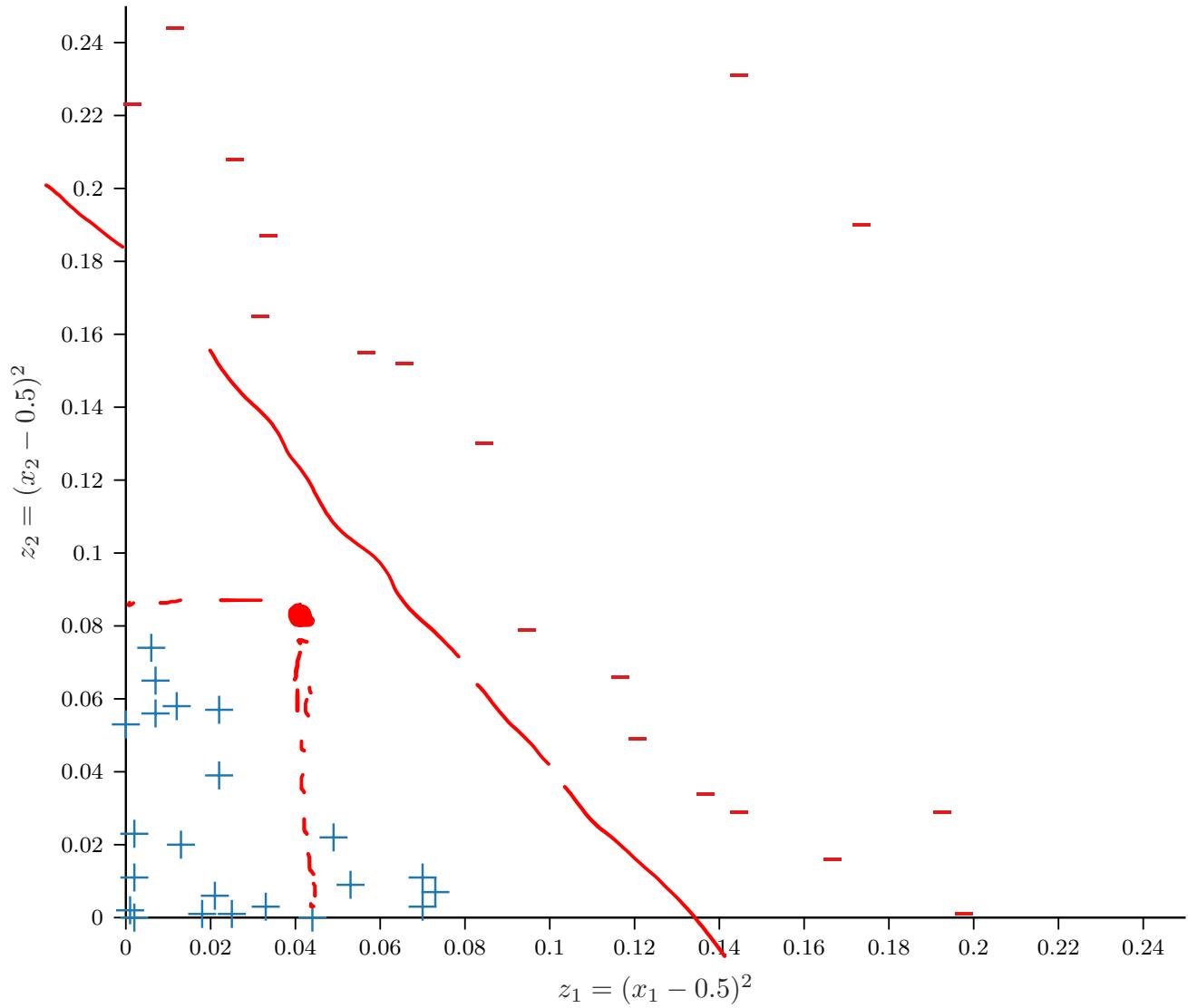
$$[x_1 = 0.7, x_2 = 0.2, y = +1] \rightarrow [z_1 = 0.04, z_2 = 0.09, y = +1]$$



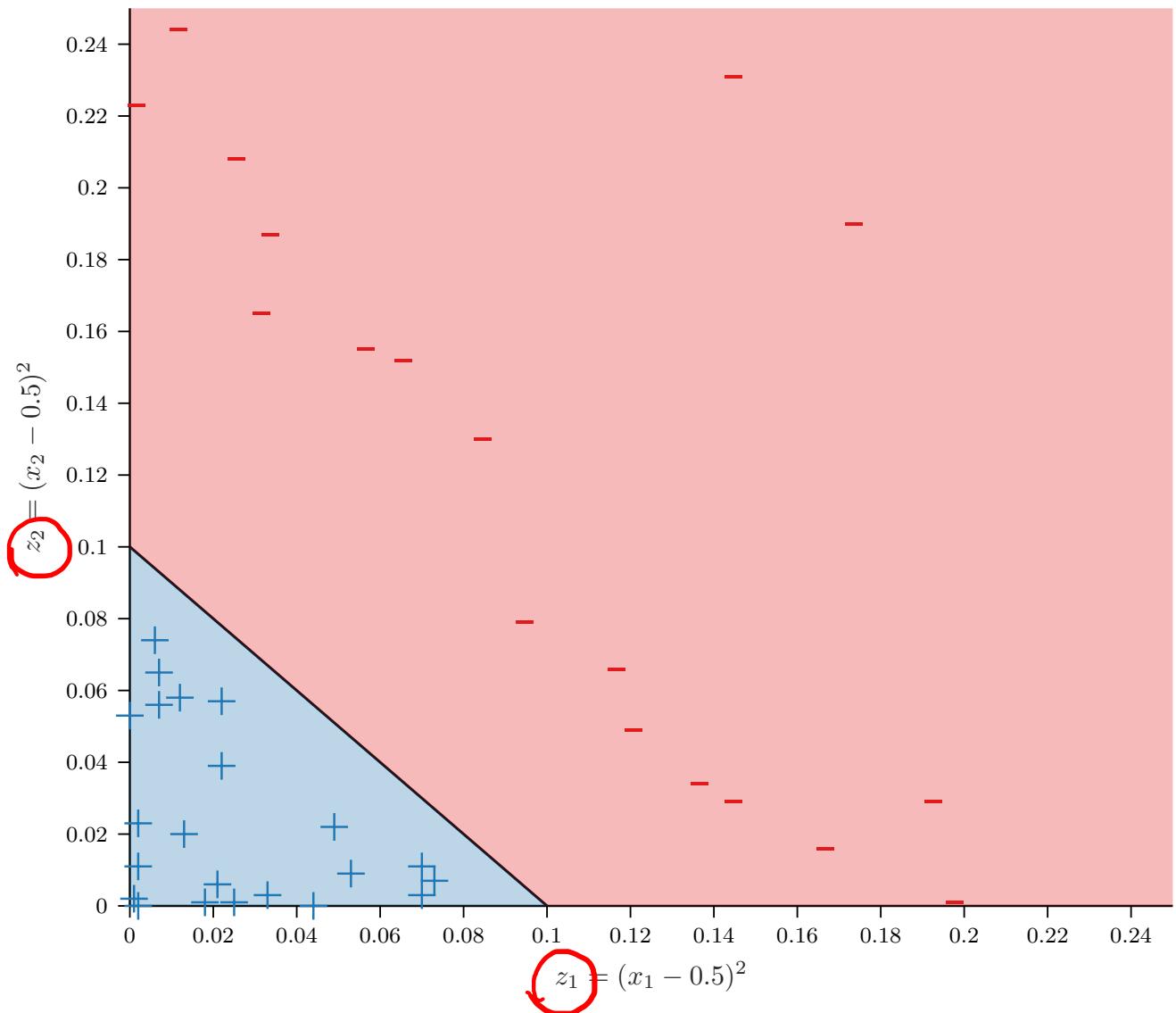
# Nonlinear Models



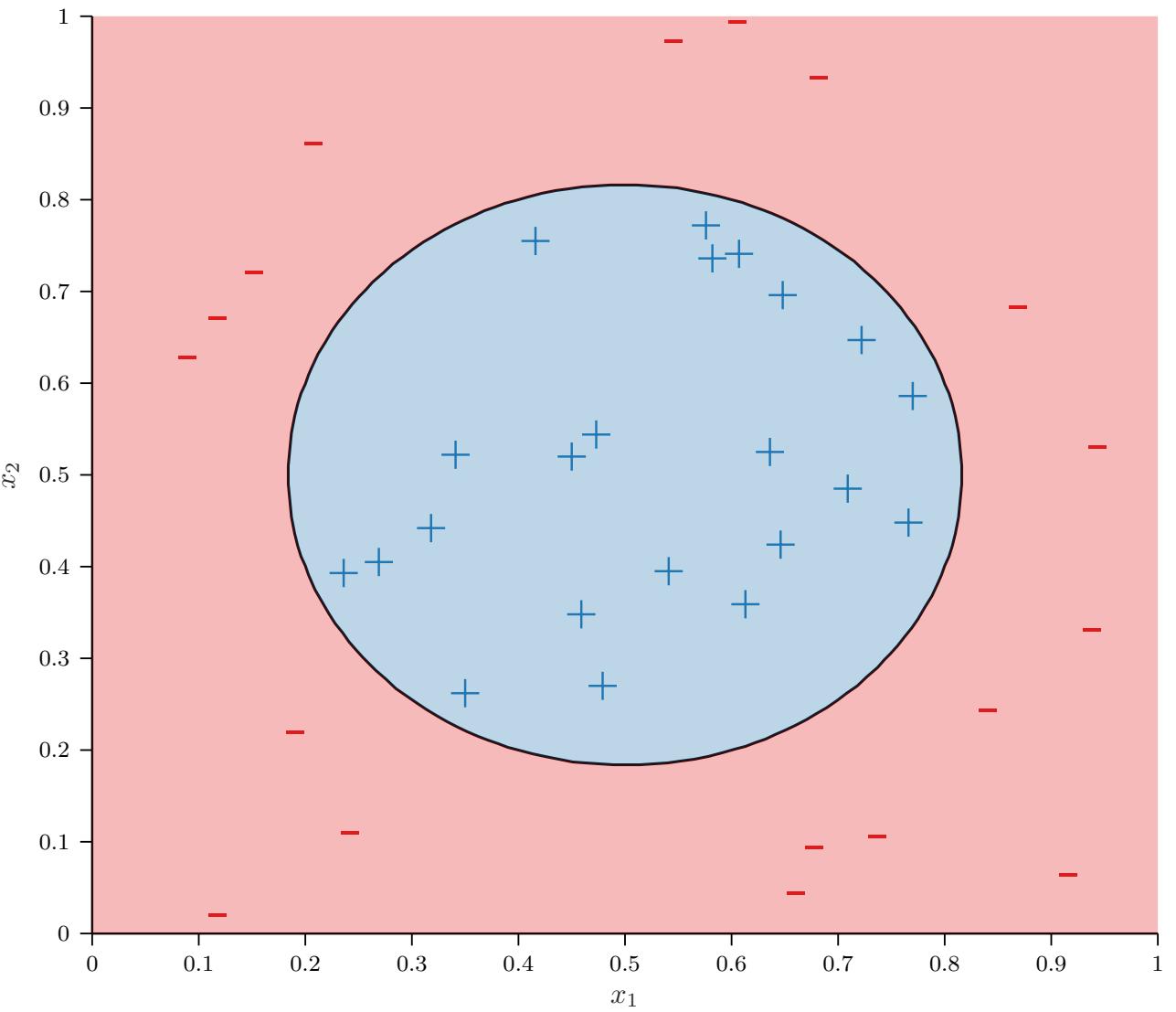
# Nonlinear Models



# Nonlinear Models



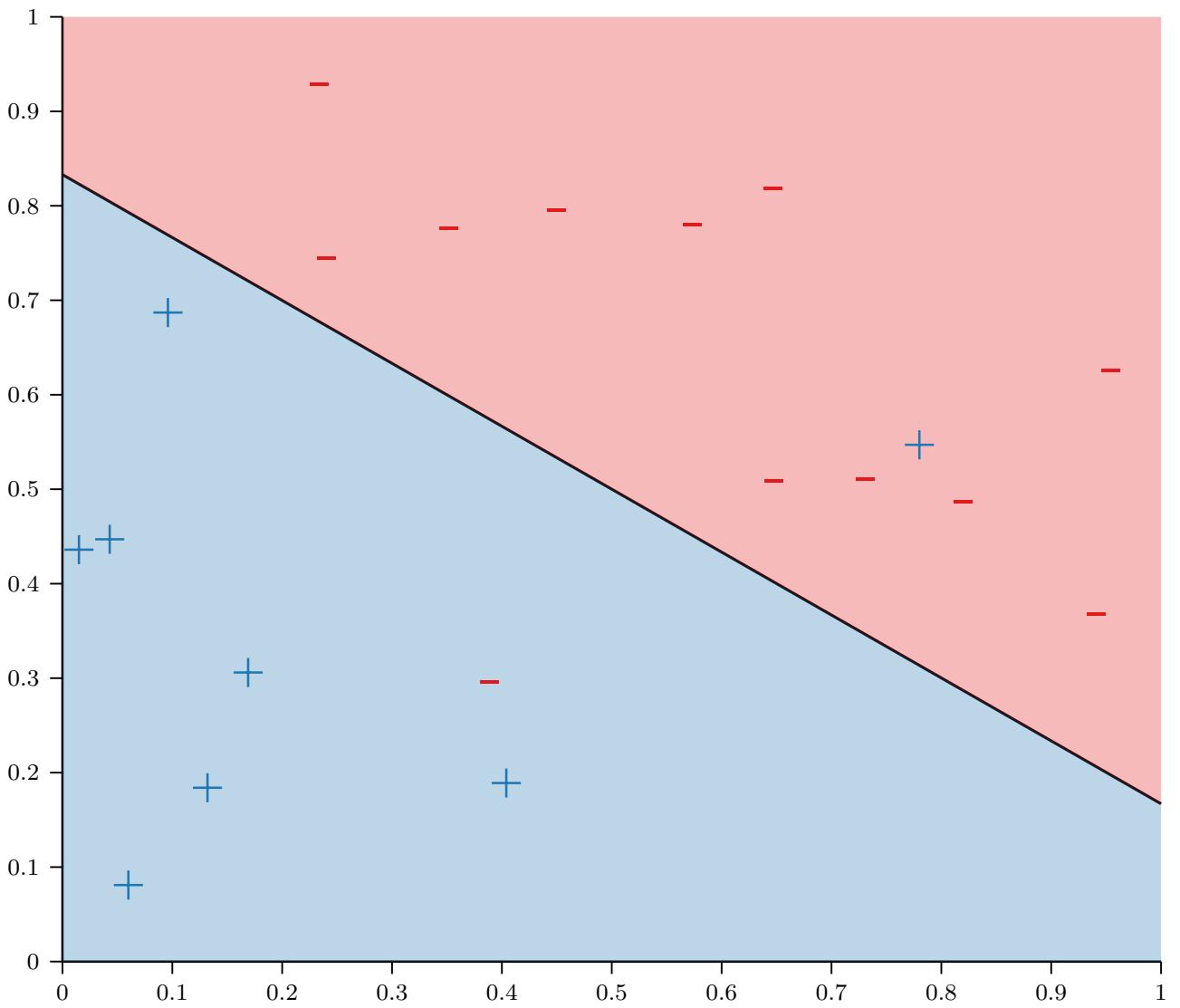
# Nonlinear Models



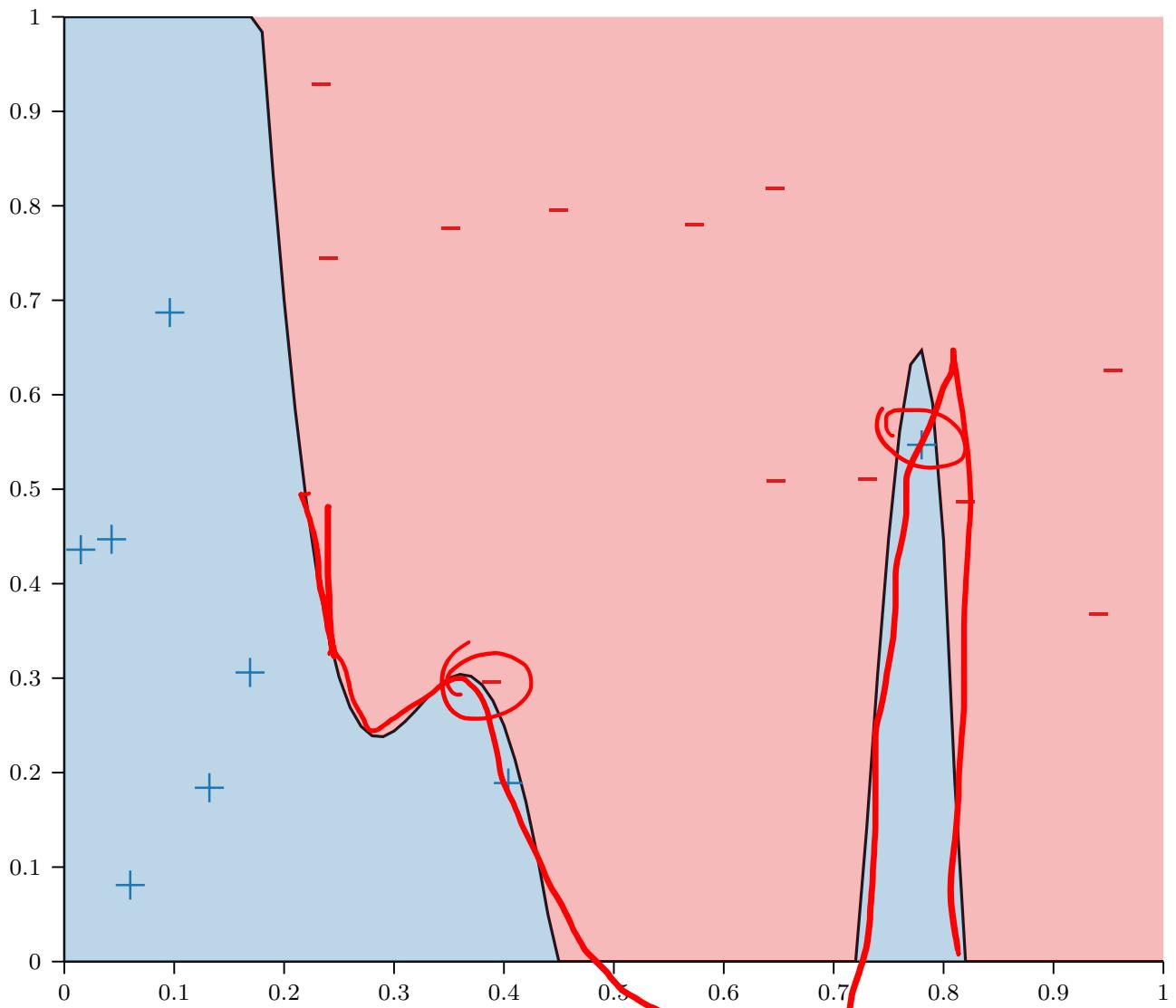
# General $Q^{th}$ -order Transforms

- #feature  $\{x_1, x_2\}$
- $\rightarrow Q$
- $\phi_{2,2}([x_1, x_2]) = [x_1, x_2, \underbrace{x_1^2}, \underbrace{x_1 x_2}, \underbrace{x_2^2}]$
  - $\phi_{2,3}([x_1, x_2]) = [x_1, x_2, x_1^2, x_1 x_2, x_2^2, \underbrace{x_1^3, x_1^2 x_2, x_1 x_2^2, x_2^3}]$
  - $\phi_{2,4}([x_1, x_2]) = [x_1, x_2, x_1^2, x_1 x_2, x_2^2, x_1^3, x_1^2 x_2, x_1 x_2^2, x_2^3, x_1^4, x_1^3 x_2, x_1^2 x_2^2, x_1 x_2^3, x_2^4]$
  - $\phi_{2,Q}$  maps a 2-dimensional input to a  $\frac{Q(Q+3)}{2}$ -dimensional output
  - Scales even worse for higher-dimensional inputs...

# Linear Models



# Nonlinear Models?



# Feature Transforms: Tradeoffs

	<b>Low-Dimensional Input Space</b>	<b>High-Dimensional Input Space</b>
<b>Training Error</b>	High	Low
<b>Generalization</b>	Good	Bad

# Feature Transforms: Experiment

- $x \in \mathbb{R}$ ,  $y \in \mathbb{R}$  and  $N = 20$
- Targets are generated by a 10<sup>th</sup>-order polynomial in  $x$  with additive Gaussian noise:

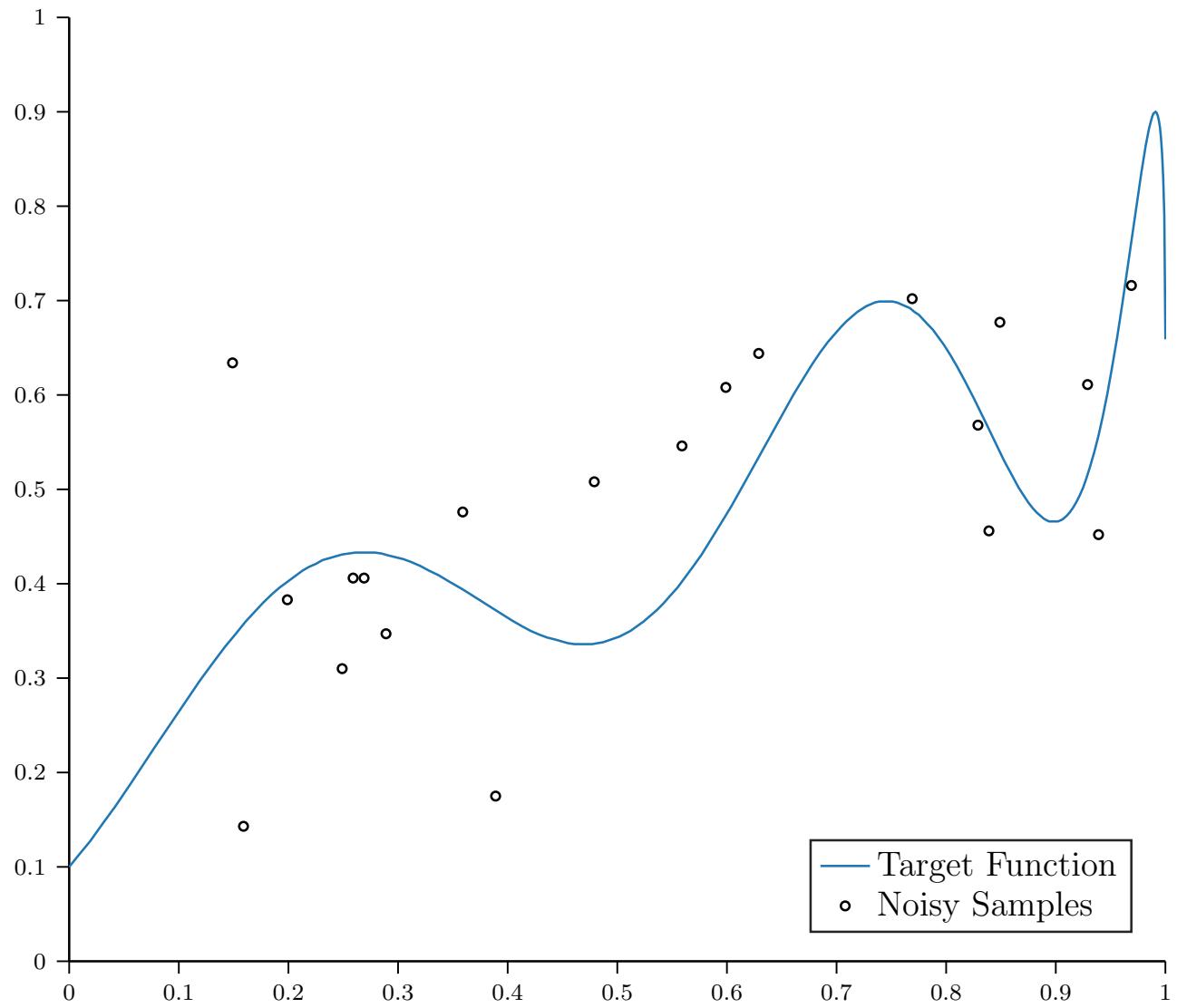
$$y = \sum_{d=0}^{10} a_d x^d + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2)$$

$= h^*(x)$

- $\mathcal{H}_2$  = 2<sup>nd</sup>-order polynomials
    - $\phi_{1,2}(x) = [x, x^2]$
  - $\mathcal{H}_{10}$  = 10<sup>th</sup>-order polynomials
    - $\phi_{1,10}(x) = [x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, x^{10}]$
- $h^*(x) \in \mathcal{H}_{10}$

# Noisy Targets

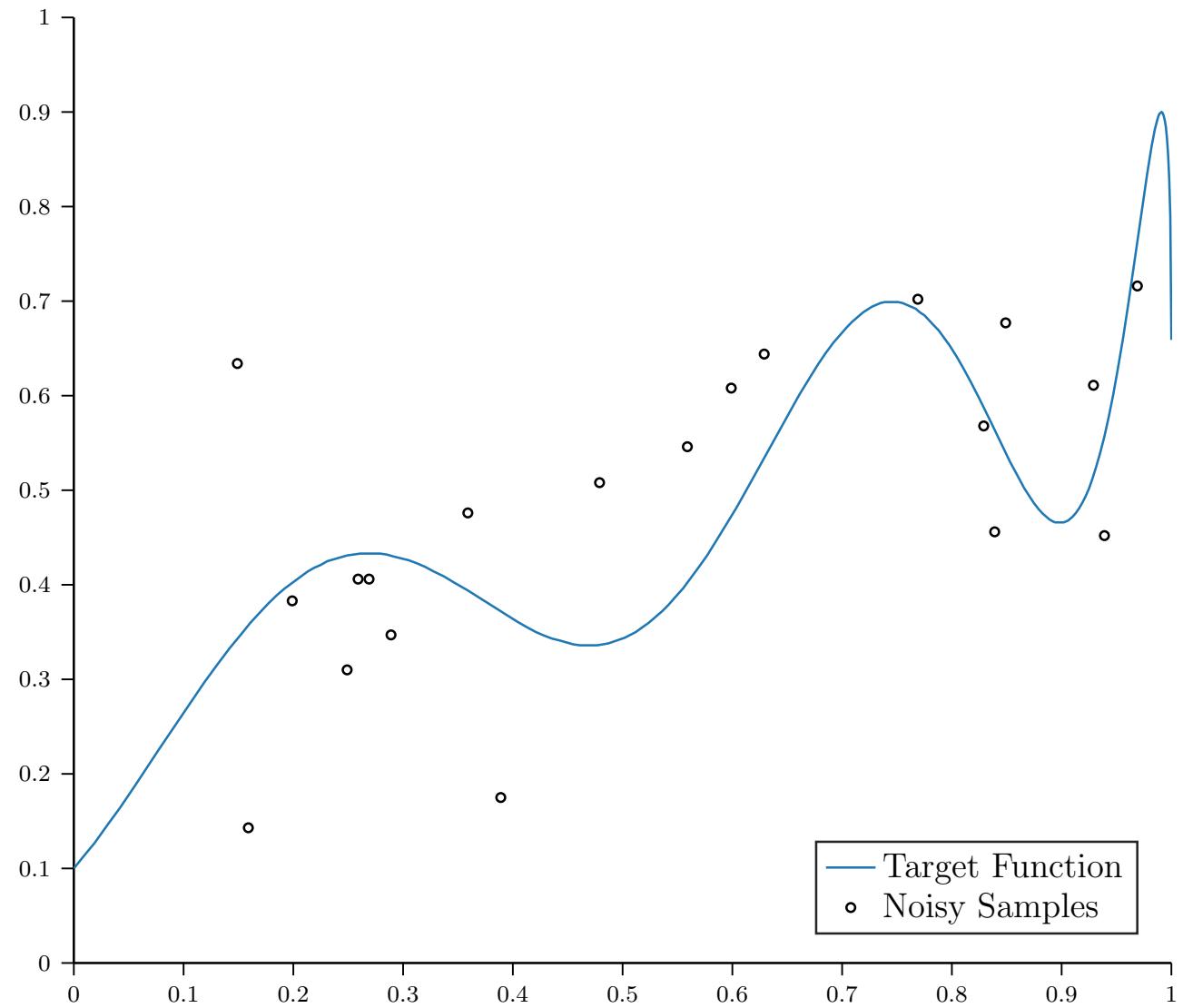
- 10-dimensional target function with additive Gaussian noise
- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomial
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomial



# Poll Question 1

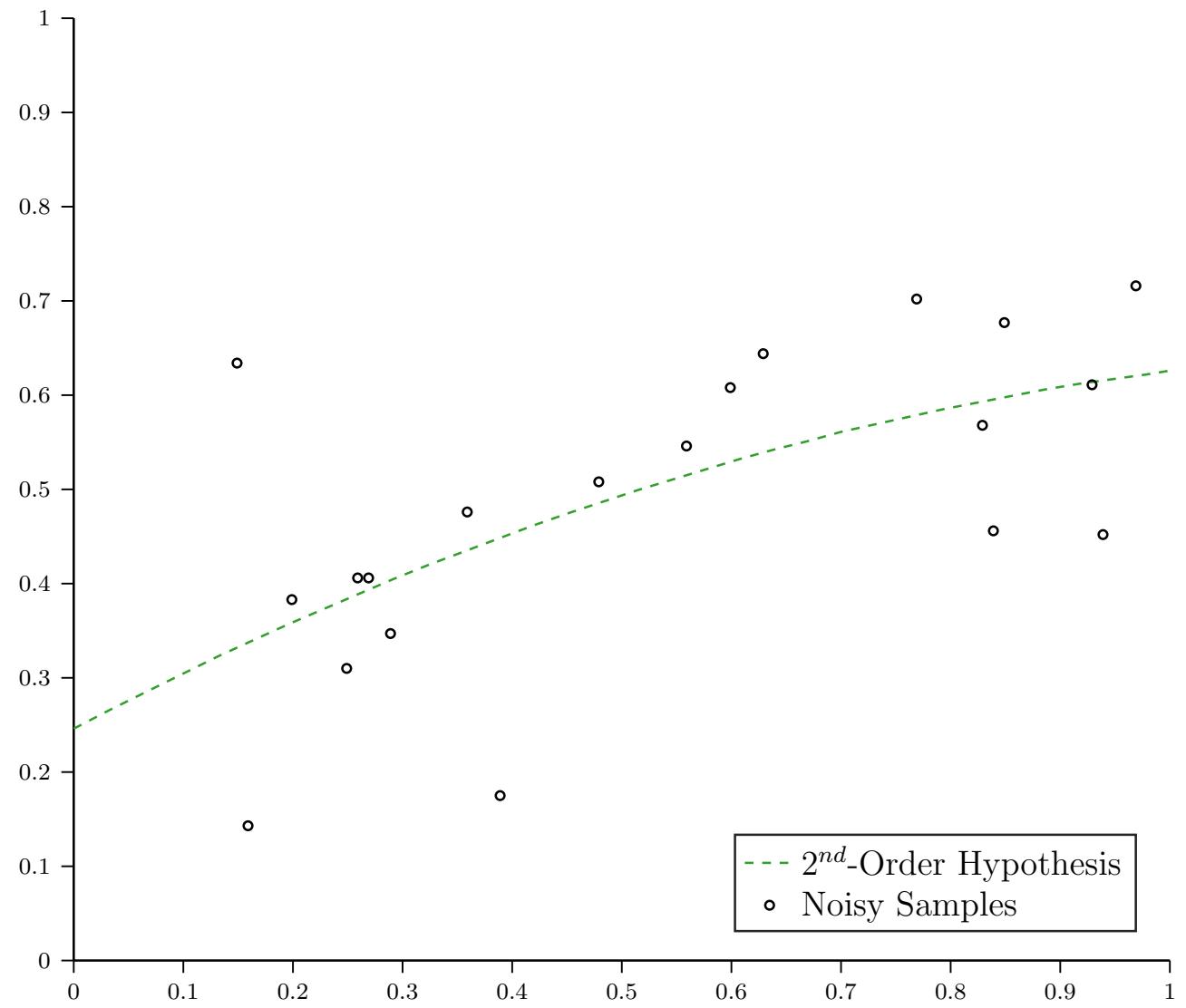
Which model do you think will have a lower true error?

- A.  $\mathcal{H}_2$
- B. TOXIC
- C.  $\mathcal{H}_{10}$



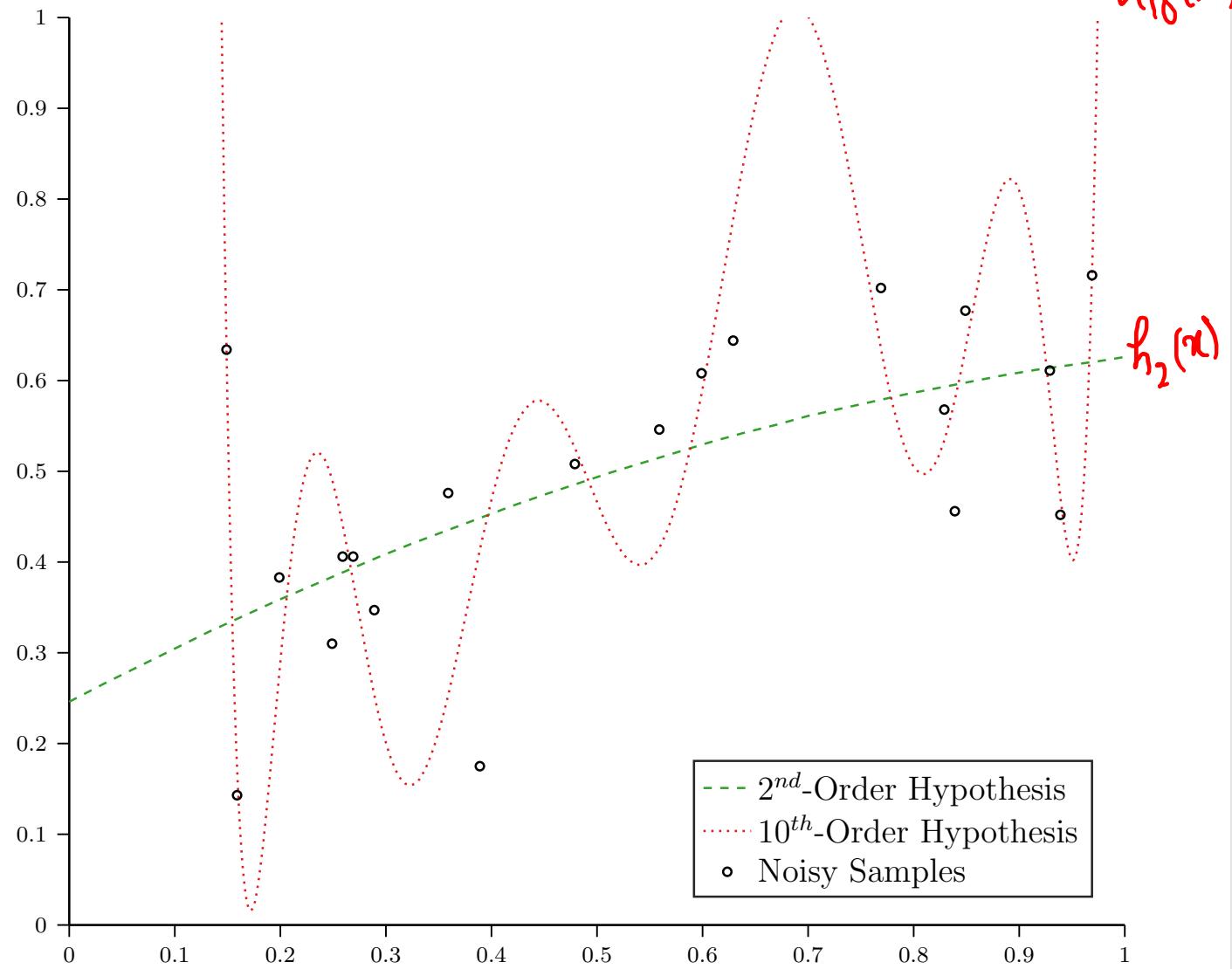
# Noisy Targets

- 10-dimensional target function with additive Gaussian noise
- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomial
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomial



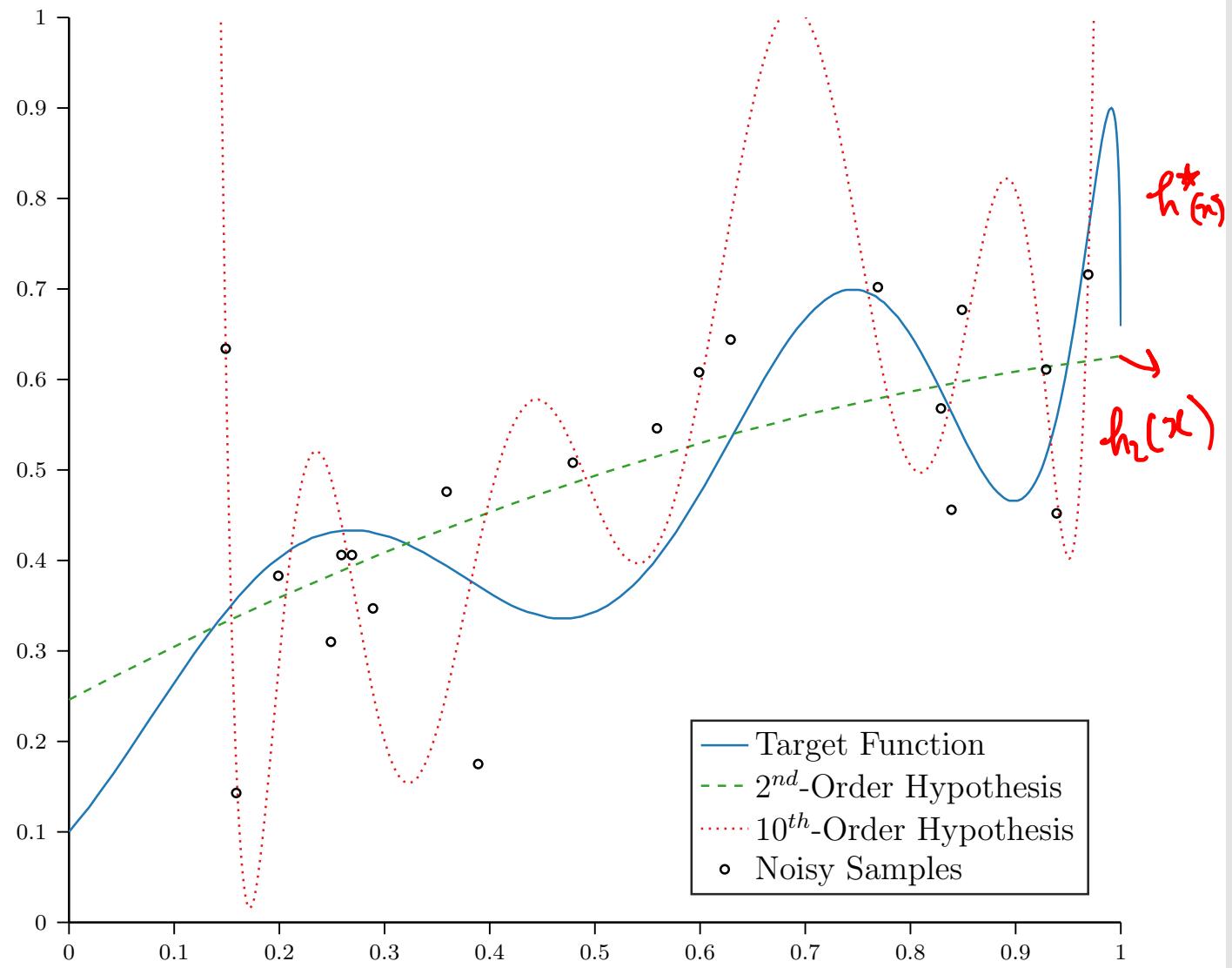
# Noisy Targets

- 10-dimensional target function with additive Gaussian noise
- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomial
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomial



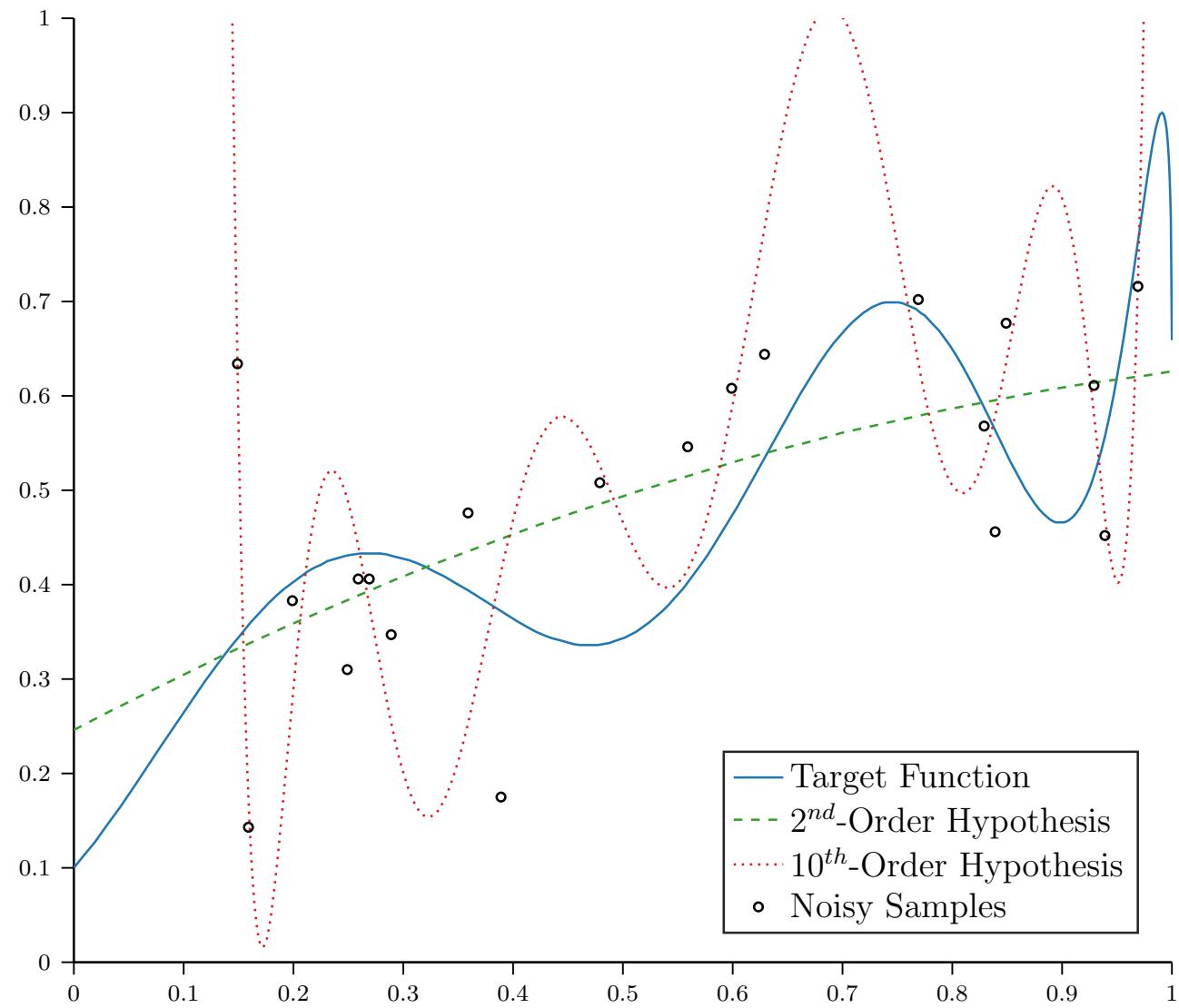
# Noisy Targets

- 10-dimensional target function with additive Gaussian noise
- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomial
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomial



# Noisy Targets

	$\mathcal{H}_2$	$\mathcal{H}_{10}$
Training Error	0.016	0.011
True Error	0.009	3797



# Feature Transforms: Experiment

- $x \in \mathbb{R}$ ,  $y \in \mathbb{R}$  and  $N = 100$
- Targets are generated by a 10<sup>th</sup>-order polynomial in  $x$  with additive Gaussian noise:

$$y = \sum_{d=0}^{10} a_d x^d + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2)$$

- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomials
  - $\phi_{1,2}(x) = [x, x^2]$
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomials
  - $\phi_{1,10}(x) = [x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, x^{10}]$

## Poll Question 2

Now which model do you think will have a lower true error?

A. TOXIC

B.  $\mathcal{H}_2$

C.  $\mathcal{H}_{10}$

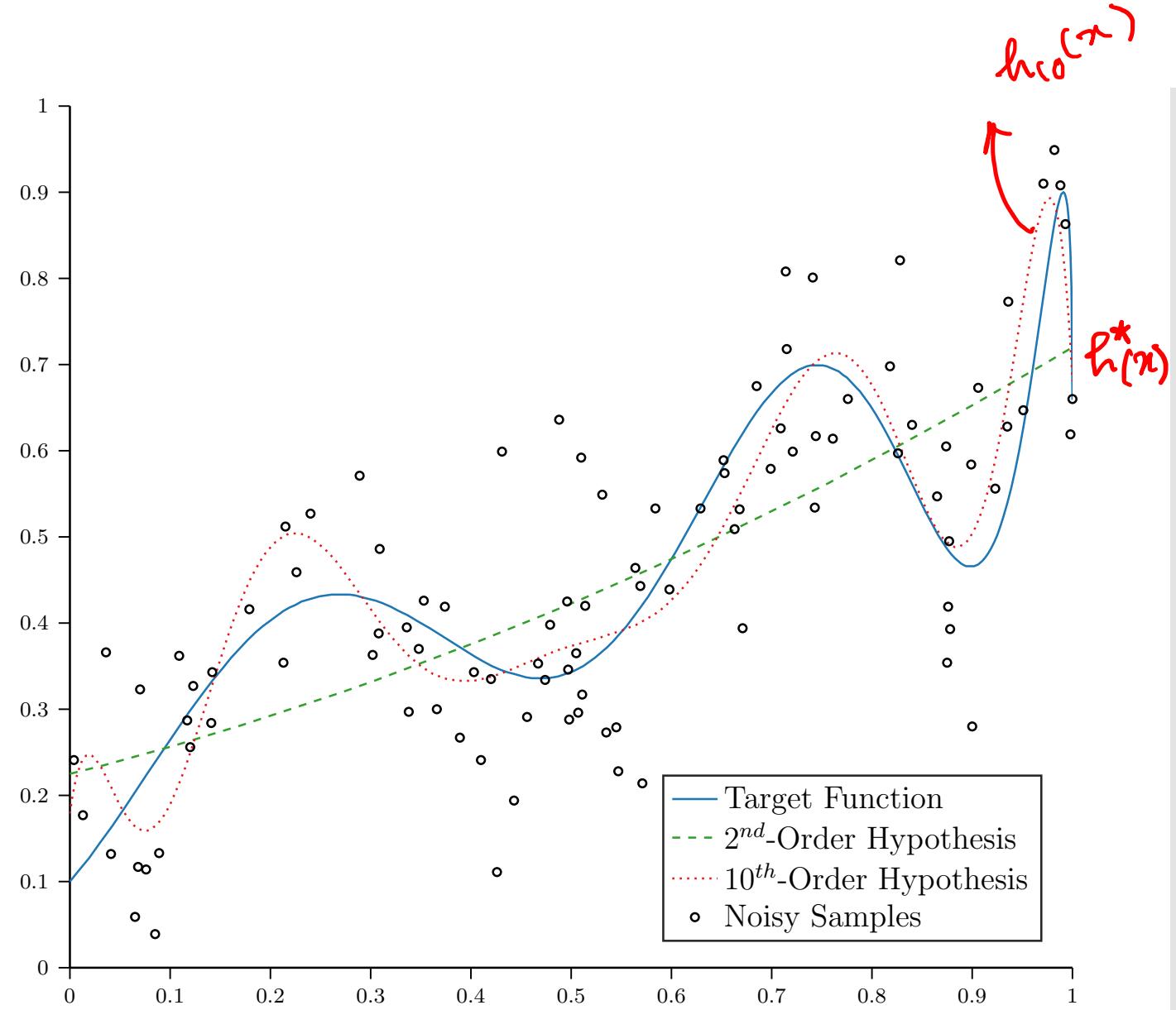
- $x \in \mathbb{R}, y \in \mathbb{R}$  and  $N = 100$
- Targets are generated by a 10<sup>th</sup>-order polynomial in  $x$  with additive Gaussian noise:

$$y = \sum_{d=0}^{10} a_d x^d + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2)$$

- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomials
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  - $\phi_{1,10}(x) = [x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, x^{10}]$

## Noisy Targets

	$\mathcal{H}_2$	$\mathcal{H}_{10}$
Training Error	0.018	0.010
True Error	0.009	0.003



# Regularization

- Constrain models to prevent them from overfitting
- Learning algorithms are optimization problems and regularization imposes constraints on the optimization

# Hard Constraints

- $\mathcal{H}_{10} = 10^{\text{th}}\text{-order polynomials}$
- $\phi_{1,10}(x) = [x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, x^{10}]$

Given  $X = \begin{bmatrix} 1 & \phi_{1,10}(x^{(1)}) \\ 1 & \phi_{1,10}(x^{(2)}) \\ \vdots & \vdots \\ 1 & \phi_{1,10}(x^{(N)}) \end{bmatrix}$  and  $y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$  find

$$\theta = [\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6, \theta_7, \theta_8, \theta_9, \theta_{10}]$$

that minimizes

$$\min_{\theta \in \mathbb{R}^n} MSE = (X\theta - y)^T (X\theta - y)$$

- Subject to

$$\theta_3 = \theta_4 = \theta_5 = \theta_6 = \theta_7 = \theta_8 = \theta_9 = \theta_{10} = 0$$

# Hard Constraints

- $\mathcal{H}_{10} = 10^{\text{th}}\text{-order polynomials}$ 
  - $\phi_{1,10}(x) = [x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, x^{10}]$
- Given  $X = \begin{bmatrix} 1 & \phi_{1,10}(x^{(1)}) \\ 1 & \phi_{1,10}(x^{(2)}) \\ \vdots & \vdots \\ 1 & \phi_{1,10}(x^{(N)}) \end{bmatrix}$  and  $y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$  find  $\theta = [\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6, \theta_7, \theta_8, \theta_9, \theta_{10}]$  that minimizes
$$\sum_{n=1}^N \left( \left( \sum_{d=0}^{10} x_d^{(n)} \theta_d \right) - y^{(n)} \right)^2$$
- Subject to
$$\theta_3 = \theta_4 = \theta_5 = \theta_6 = \theta_7 = \theta_8 = \theta_9 = \theta_{10} = 0$$

# Hard Constraints

- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomials
  - $\phi_{1,10}(x) = [x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, x^{10}]$
- Given  $X = \begin{bmatrix} 1 & \phi_{1,10}(x^{(1)}) \\ 1 & \phi_{1,10}(x^{(2)}) \\ \vdots & \vdots \\ 1 & \phi_{1,10}(x^{(N)}) \end{bmatrix}$  and  $y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$  find  $\theta = [\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6, \theta_7, \theta_8, \theta_9, \theta_{10}]$  that minimizes
$$\sum_{n=1}^N \left( \left( \sum_{d=0}^2 x_d^{(n)} \theta_d \right) - y^{(n)} \right)^2$$
- Subject to nothing!

# Hard Constraints

- $\mathcal{H}_2 = 2^{\text{nd}}\text{-order polynomials}$ 
  - $\phi_{1,2}(x) = [x, x^2]$
- Given  $X = \begin{bmatrix} 1 & \phi_{1,2}(x^{(1)}) \\ 1 & \phi_{1,2}(x^{(2)}) \\ \vdots & \vdots \\ 1 & \phi_{1,2}(x^{(N)}) \end{bmatrix}$  and  $y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$  find  
 $\theta = [\theta_0, \theta_1, \theta_2]$   
that minimizes
$$(X\theta - y)^T(X\theta - y)$$
- Subject to nothing!

# Soft Constraints

- More generally,  $\phi$  can be any nonlinear transformation, e.g., exp, log, sin, sqrt, etc...

Given  $X = \begin{bmatrix} 1 & \phi_1(\mathbf{x}^{(1)}) & \dots & \phi_m(\mathbf{x}^{(1)}) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \phi_1(\mathbf{x}^{(N)}) & \dots & \phi_m(\mathbf{x}^{(N)}) \end{bmatrix}$  and  $\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$ ,  
find  $\boldsymbol{\theta}$  that minimizes

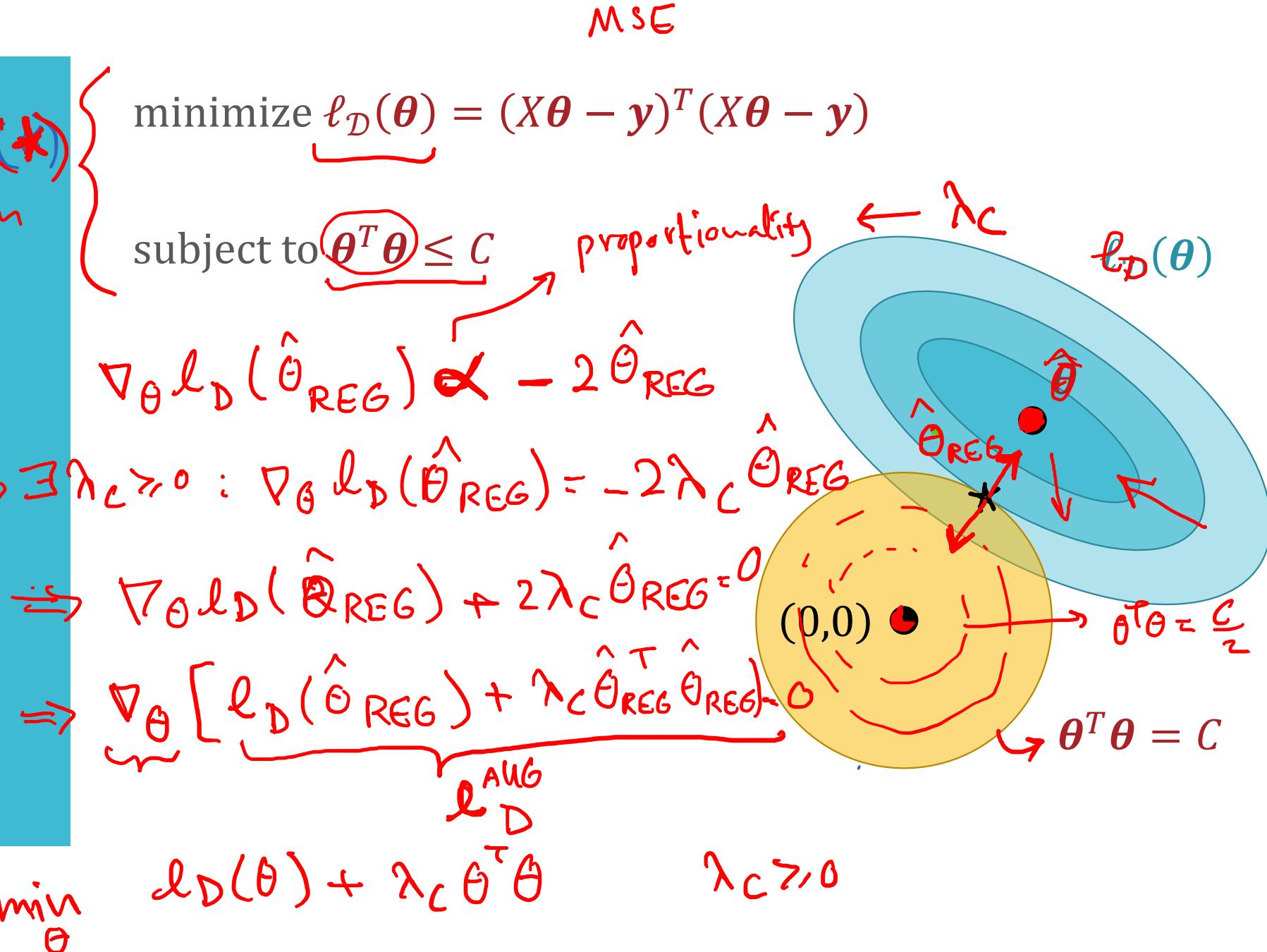
$$\min \text{MSE} = \underbrace{(X\boldsymbol{\theta} - \mathbf{y})^T(X\boldsymbol{\theta} - \mathbf{y})}_{\text{MSE}}$$

- Subject to:

*constraint*  $\underbrace{\|\boldsymbol{\theta}\|_2^2}_{\text{constraint}} = \boldsymbol{\theta}^T \boldsymbol{\theta} = \sum_{d=0}^D \theta_d^2 \leq C$

Soft  
Constraints

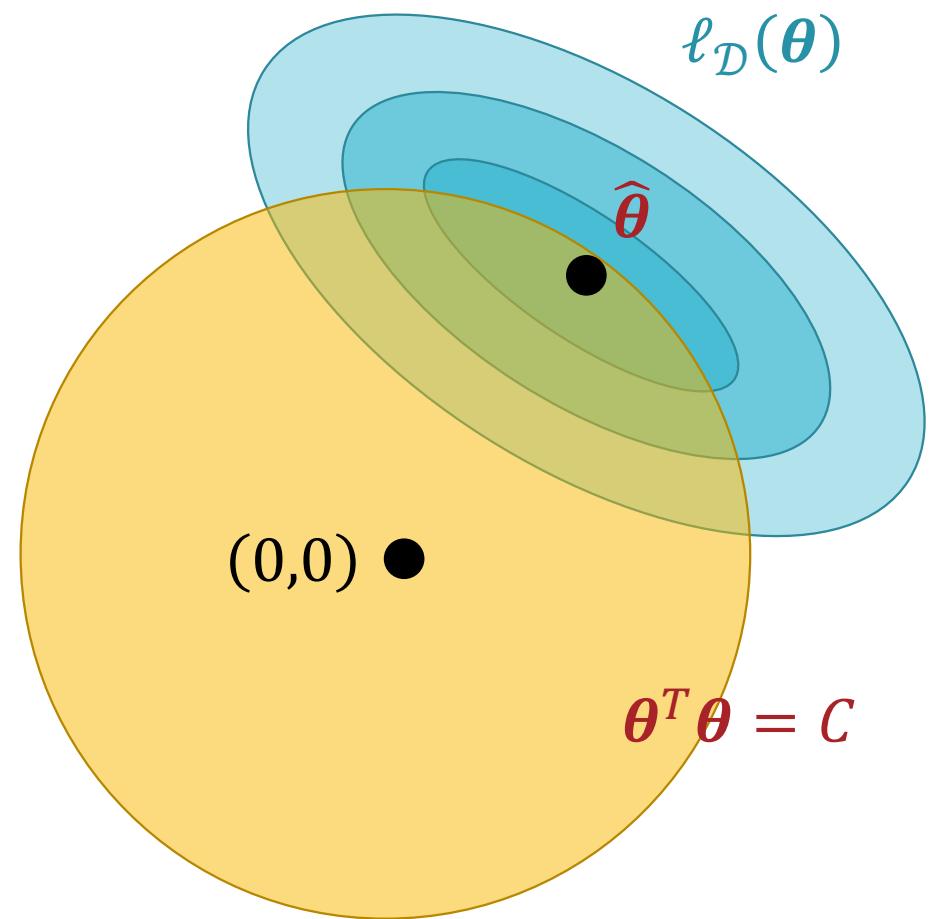
constrained (\*)  
optimization



# Soft Constraints

$$\text{minimize } \ell_{\mathcal{D}}(\boldsymbol{\theta}) = (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^T(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$$

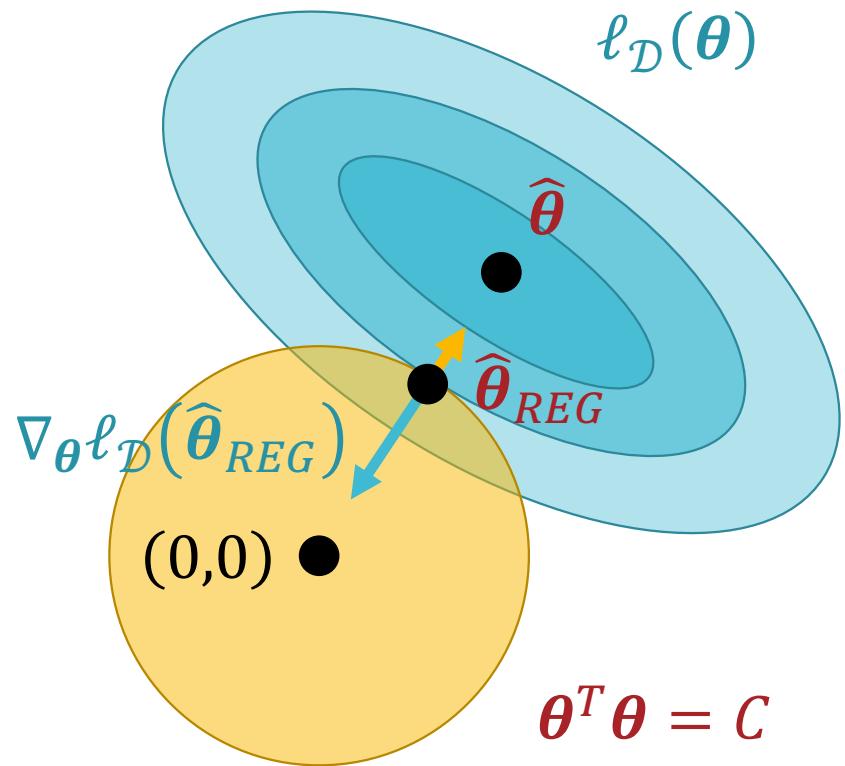
$$\text{subject to } \boldsymbol{\theta}^T \boldsymbol{\theta} \leq C$$



# Soft Constraints

minimize  $\ell_{\mathcal{D}}(\boldsymbol{\theta}) = (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^T(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$

subject to  $\boldsymbol{\theta}^T \boldsymbol{\theta} \leq C$



# Soft Constraints: Solving for $\hat{\theta}_{REG}$

$$\text{minimize } \ell_{\mathcal{D}}(\boldsymbol{\theta}) = (X\boldsymbol{\theta} - y)^T(X\boldsymbol{\theta} - y)$$

$$\text{subject to } \boldsymbol{\theta}^T \boldsymbol{\theta} \leq C$$

$\Updownarrow$

$$\text{minimize } \underbrace{\ell_{\mathcal{D}}^{AUG}(\boldsymbol{\theta})}_{\ell_{\mathcal{D}}(\boldsymbol{\theta}) + \lambda_C \boldsymbol{\theta}^T \boldsymbol{\theta}}$$

# Ridge Regression

$$MSE = (\hat{X}^T \theta - Y)^T (\hat{X}^T \theta - Y)$$

$$\text{minimize } \ell_D^{AUG}(\theta) = \ell_D(\theta) + \lambda_C \theta^T \theta$$

$$\nabla \ell^{AUG}(\hat{\theta}_{REG}) = \cancel{\frac{1}{2} X^T X \hat{\theta}_{REG}} - \cancel{\frac{1}{2} X^T Y} + \cancel{\frac{1}{2} \lambda_C \hat{\theta}_{REG}} = 0$$

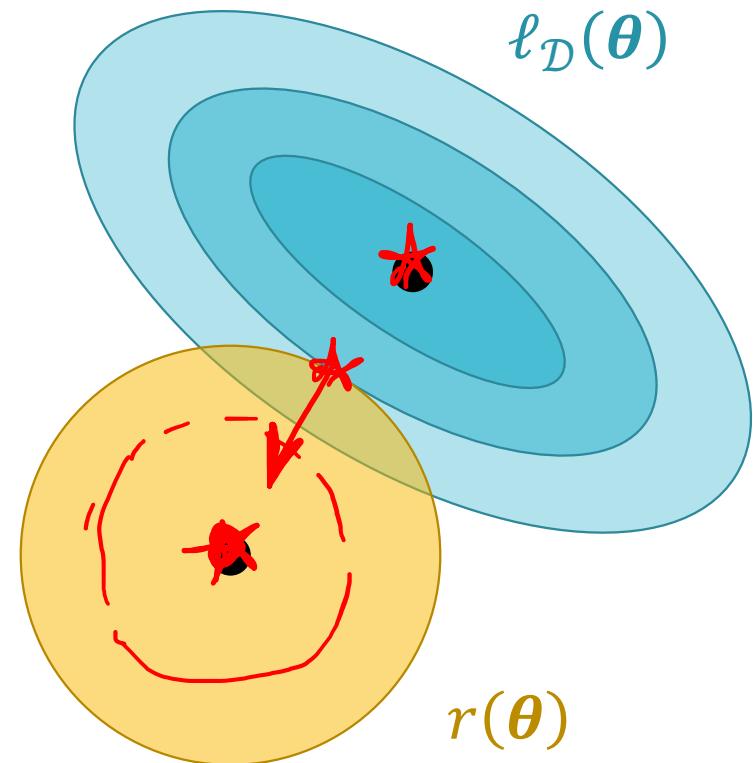
$$\Rightarrow \cancel{X^T X \hat{\theta}_{REG}} + \cancel{\lambda_C \hat{\theta}_{REG}} = X^T Y$$

$$\Rightarrow \underbrace{(X^T X + \lambda_C I)}_{\text{Matrix}} \hat{\theta}_{REG} = X^T Y$$

$$\Rightarrow \boxed{\hat{\theta}_{REG} = (X^T X + \lambda_C I)^{-1} X^T Y}$$

## Poll Question 3

- Suppose we are minimizing  $\ell_D^{AUG}(\theta) = \ell_D(\theta) + \lambda_C r(\theta)$ .  
As  $\lambda_C$  increases, the minimum of  $\ell_D^{AUG}$  ...
- A. ... moves towards the midpoint of  $\ell_D$  and  $r$
- B. ... moves towards the minimum of  $\ell_D$
- C. ... moves towards the minimum of  $r$
- D. ... moves towards the vector of all infinities
- E. ... moves towards the vector of all ones
- ~~F. ... stays the same~~

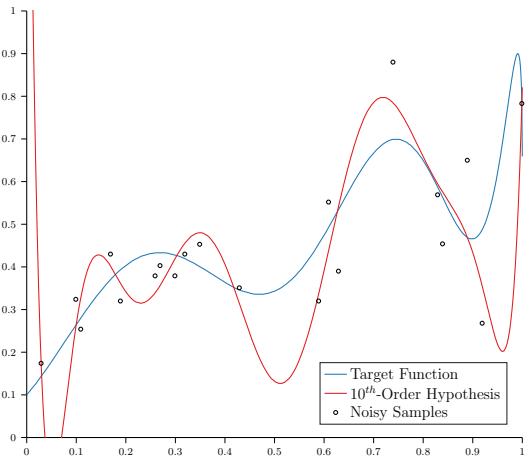


## Regularization: Q & A

- Should we regularize the bias/intercept parameter,  $\theta_0$ ?
- Is feature scale a concern with regularization?

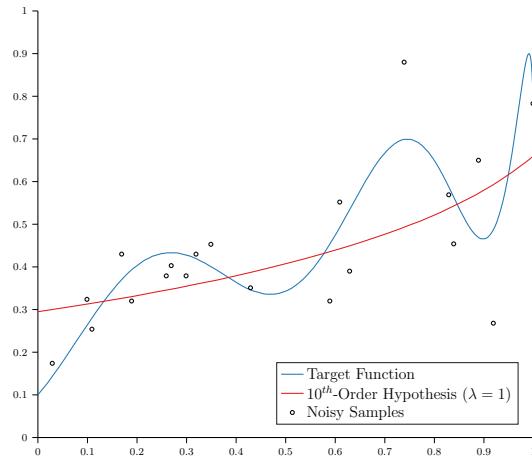
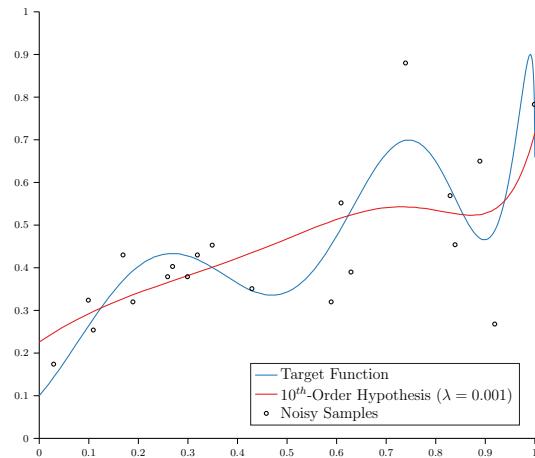
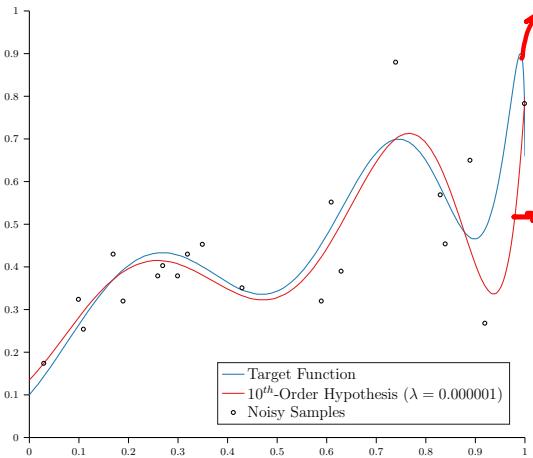
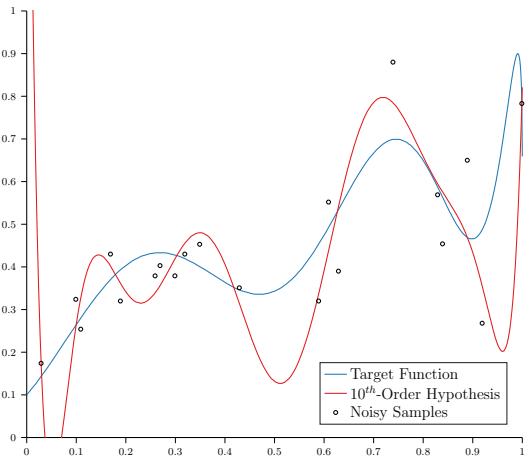
# Regularization: Best Practices

- Should we regularize the bias/intercept parameter,  $\theta_0$ ?
  - No!
  - Regularizers typically avoid penalizing this term so that our classifiers can adapt to shifts in the  $y$  values
- Is feature scale a concern with regularization?
  - Yes!
  - Features at dramatically different scales might have vastly different coefficient values
  - When using regularization, it is common to *standardize* the features first by subtracting the mean and dividing by the standard deviation



# Ridge Regression

- 10-dimensional target function with additive Gaussian noise
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomial



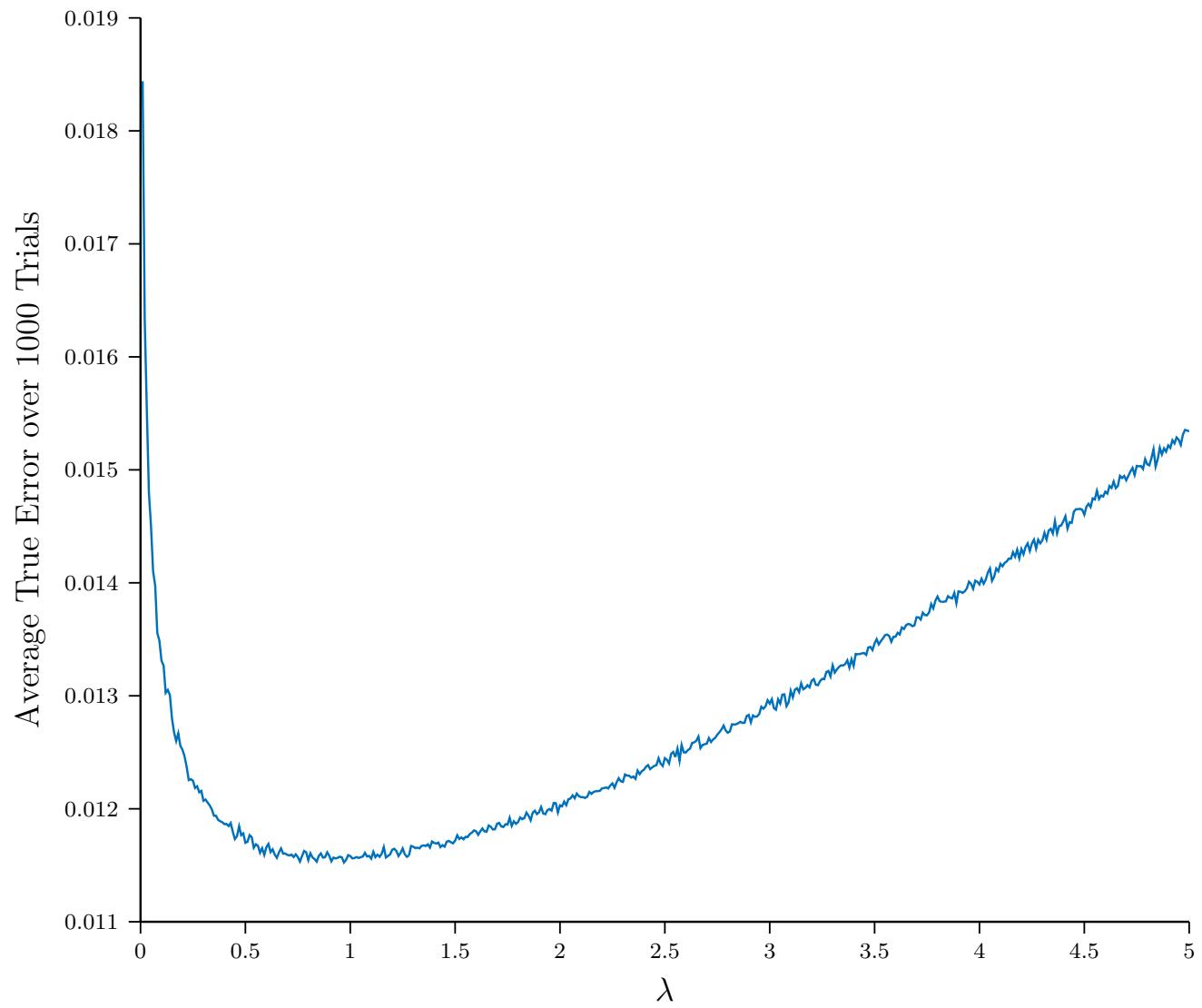
# Ridge Regression

$$\lambda_c = 0$$

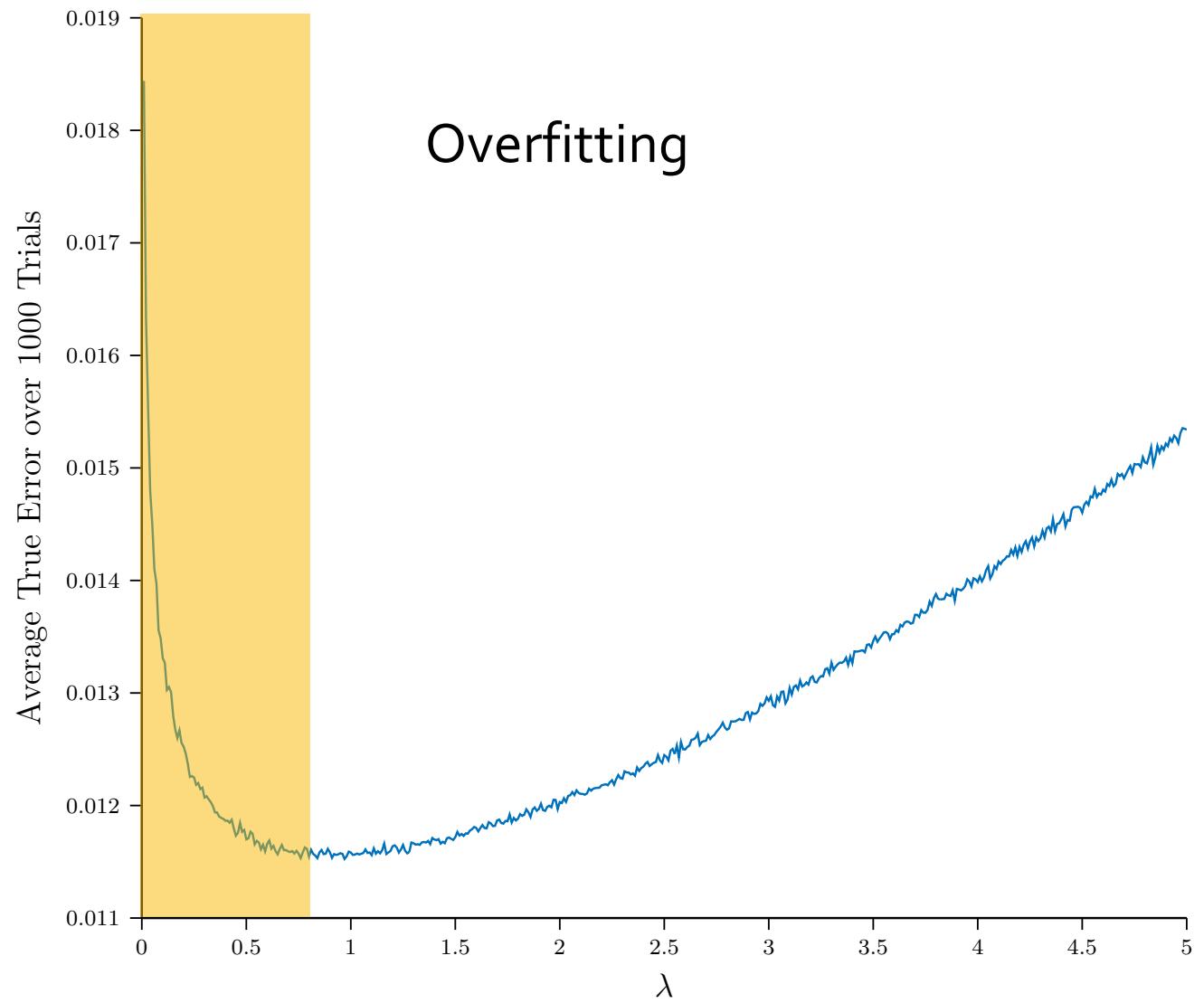
True  
Error  
0.059

Overfit

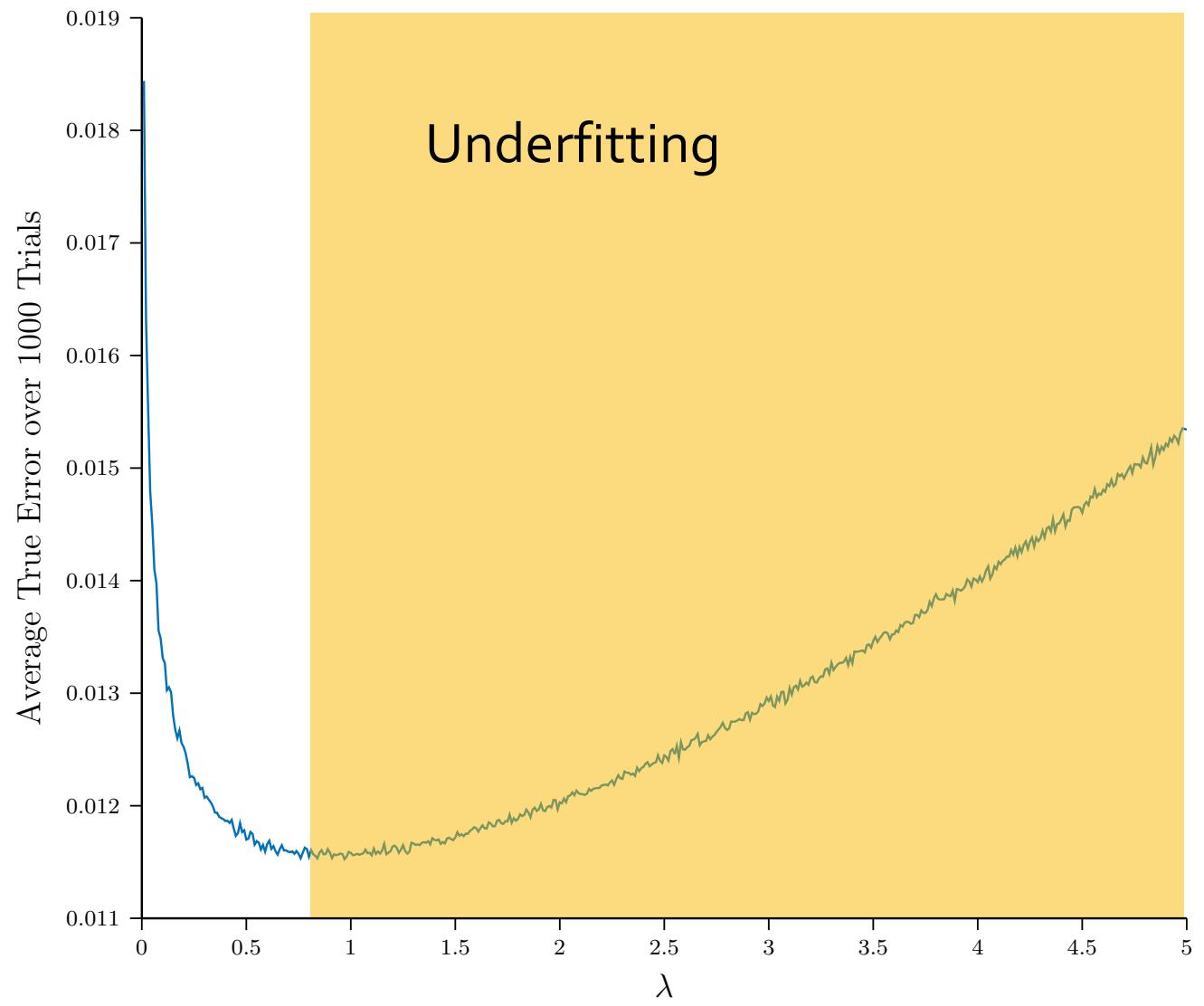
# Setting $\lambda$



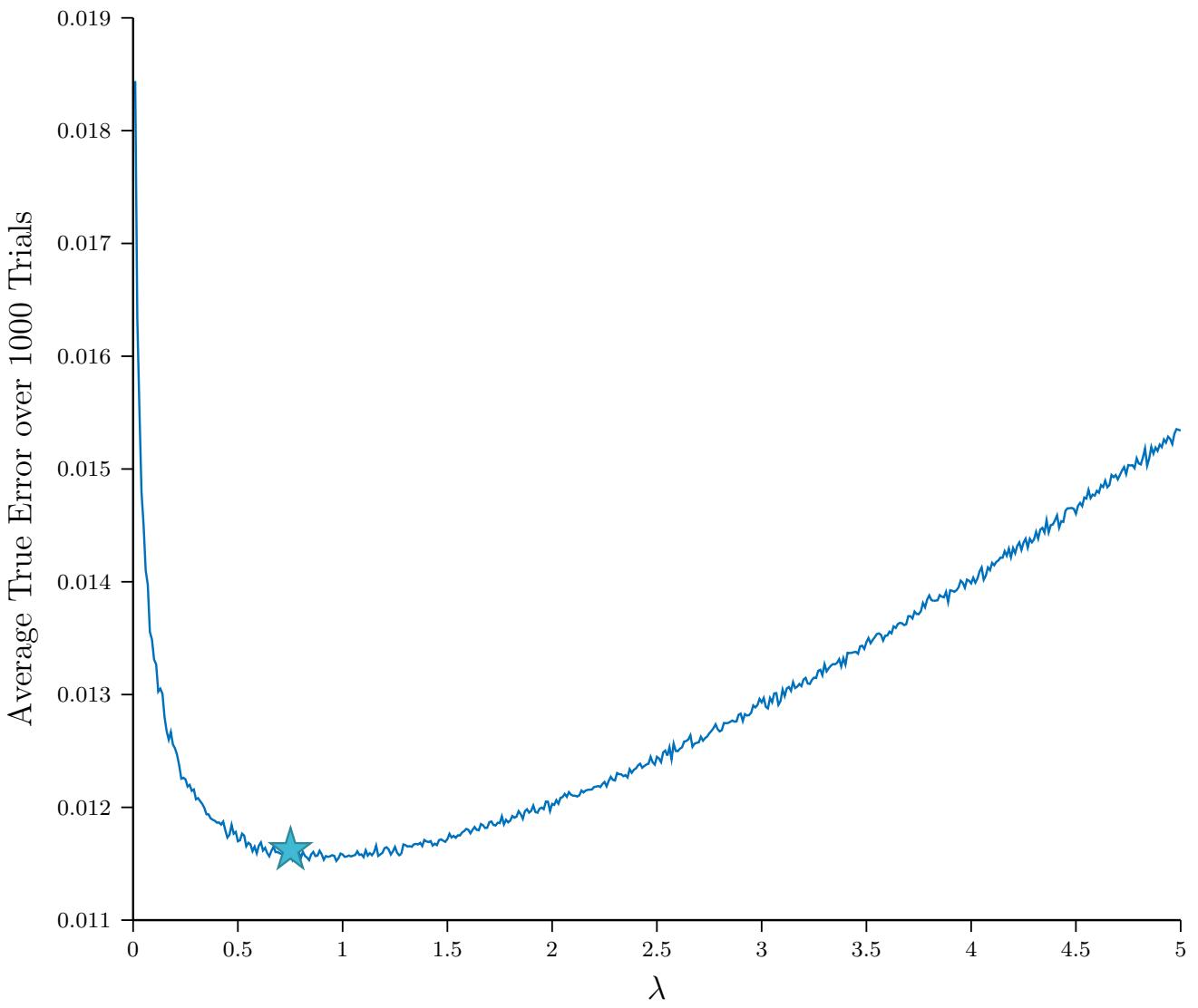
# Setting $\lambda$



# Setting $\lambda$

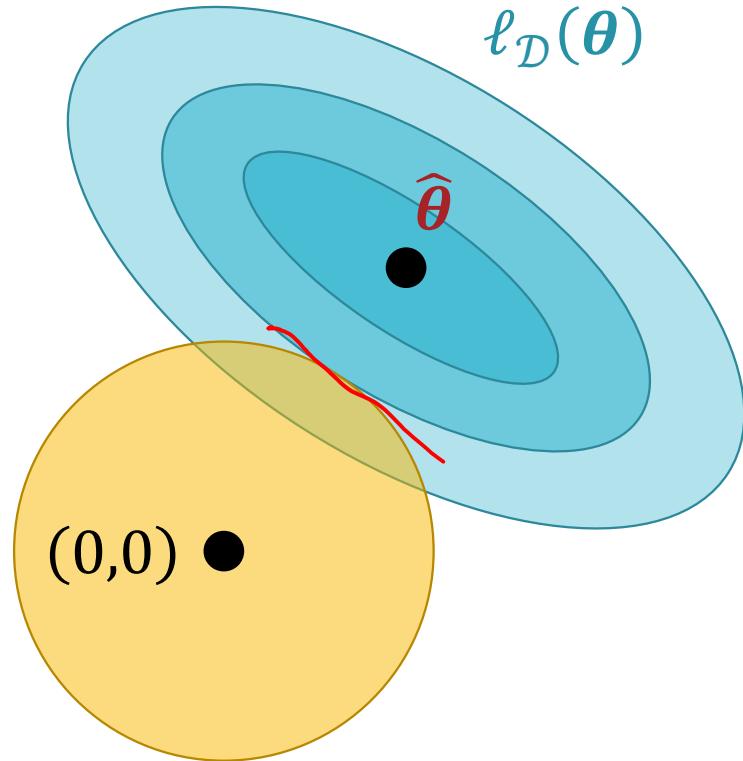


# Setting $\lambda$

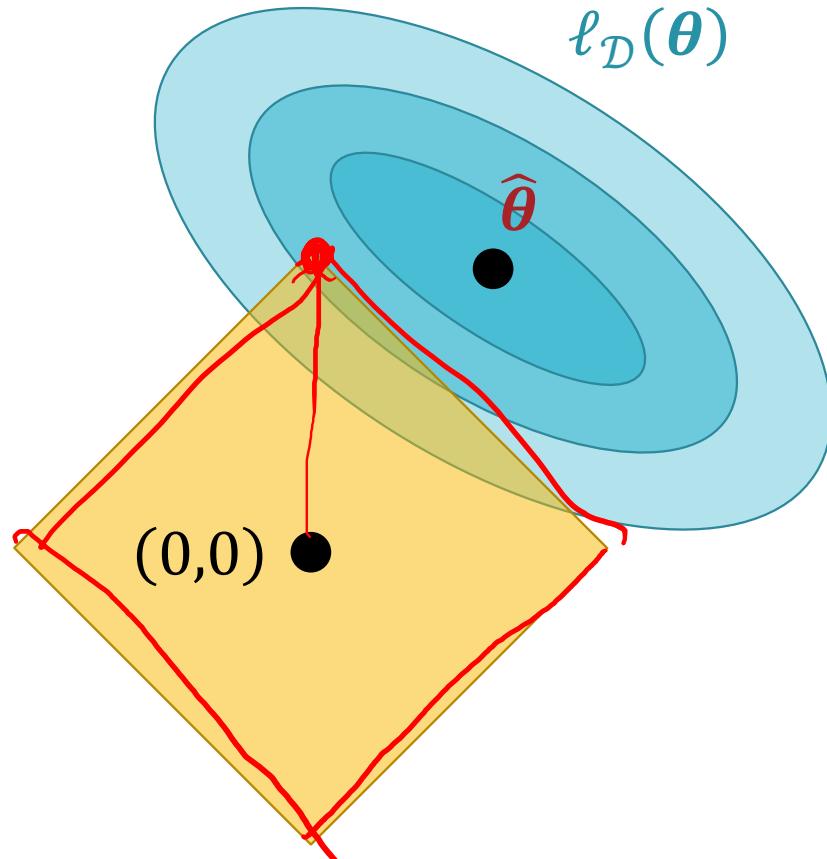


## Other Regularizers

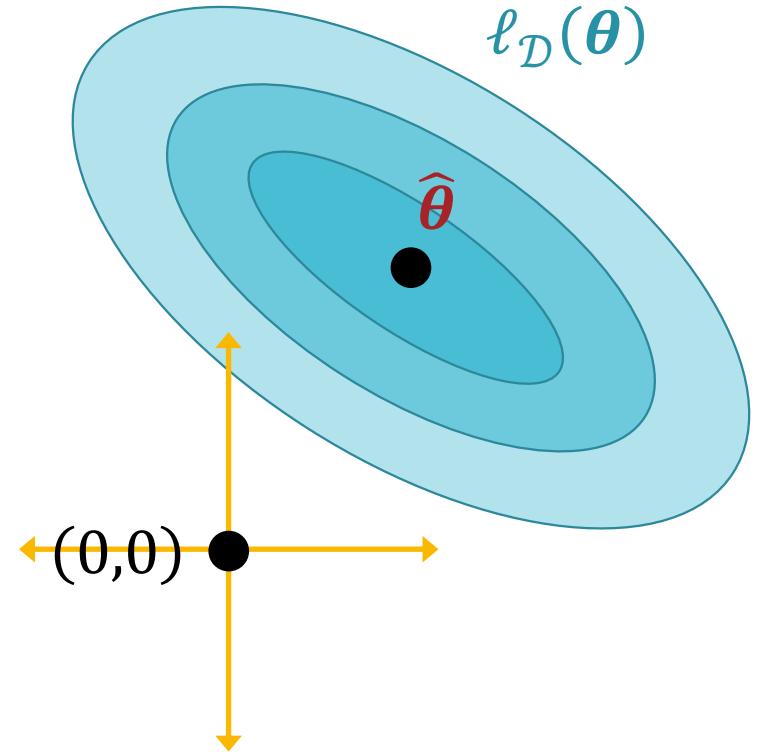
$\ell_{\mathcal{D}}(\boldsymbol{\theta}) + \lambda r(\boldsymbol{\theta})$			
Ridge or $L2$	$r(\boldsymbol{\theta}) = \underbrace{\ \boldsymbol{\theta}\ _2^2}_{\sum_{d=0}^D \theta_d^2}$		Encourages small weights
Lasso or $L1$	$r(\boldsymbol{\theta}) = \underbrace{\ \boldsymbol{\theta}\ _1}_{\sum_{d=0}^D  \theta_d }$		Encourages sparsity
$L0$	$r(\boldsymbol{\theta}) = \underbrace{\ \boldsymbol{\theta}\ _0}_{\sum_{d=0}^D \mathbb{1}(\theta_d \neq 0)}$		Encourages sparsity (intractable)



Ridge or  $L2$



Lasso or  $L1$



$L0$

## Other Regularizers

# Regularization Learning Objectives

You should be able to...

- Identify when a model is overfitting
- Add a regularizer to an existing objective in order to combat overfitting
- Explain why we should not regularize the bias term
- Convert linearly inseparable dataset to a linearly separable dataset in higher dimensions