

10-301/601: Introduction to Machine Learning

Lecture 10 – Regularization

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10/2/23

Front Matter

- Announcements:
 - HW4 released 9/29, due 10/9 at 11:59 PM

Recall: Logistic Regression

- Model:

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \begin{cases} \sigma(\boldsymbol{\theta}^T \mathbf{x}) & \text{if } y = 1 \\ 1 - \sigma(\boldsymbol{\theta}^T \mathbf{x}) & \text{if } y = 0 \end{cases}$$

where $\sigma(z) = 1/(1 + \exp(-z))$

- Derivatives

$$\begin{aligned} \frac{\partial J^{(i)}}{\partial \theta_m} &= \frac{\partial}{\partial \theta_m} (-\log p(y^{(i)}|\mathbf{x}^{(i)}, \boldsymbol{\theta})) \\ &\vdots \\ &= -\left(y^{(i)} - \sigma(\boldsymbol{\theta}^T \mathbf{x}^{(i)})\right) \mathbf{x}_m^{(i)} \end{aligned}$$

- Optimization: use GD or SGD;
logistic regression does not permit a
closed form solution

- Objective: minimize the negative
conditional log-likelihood

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

- Gradients

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

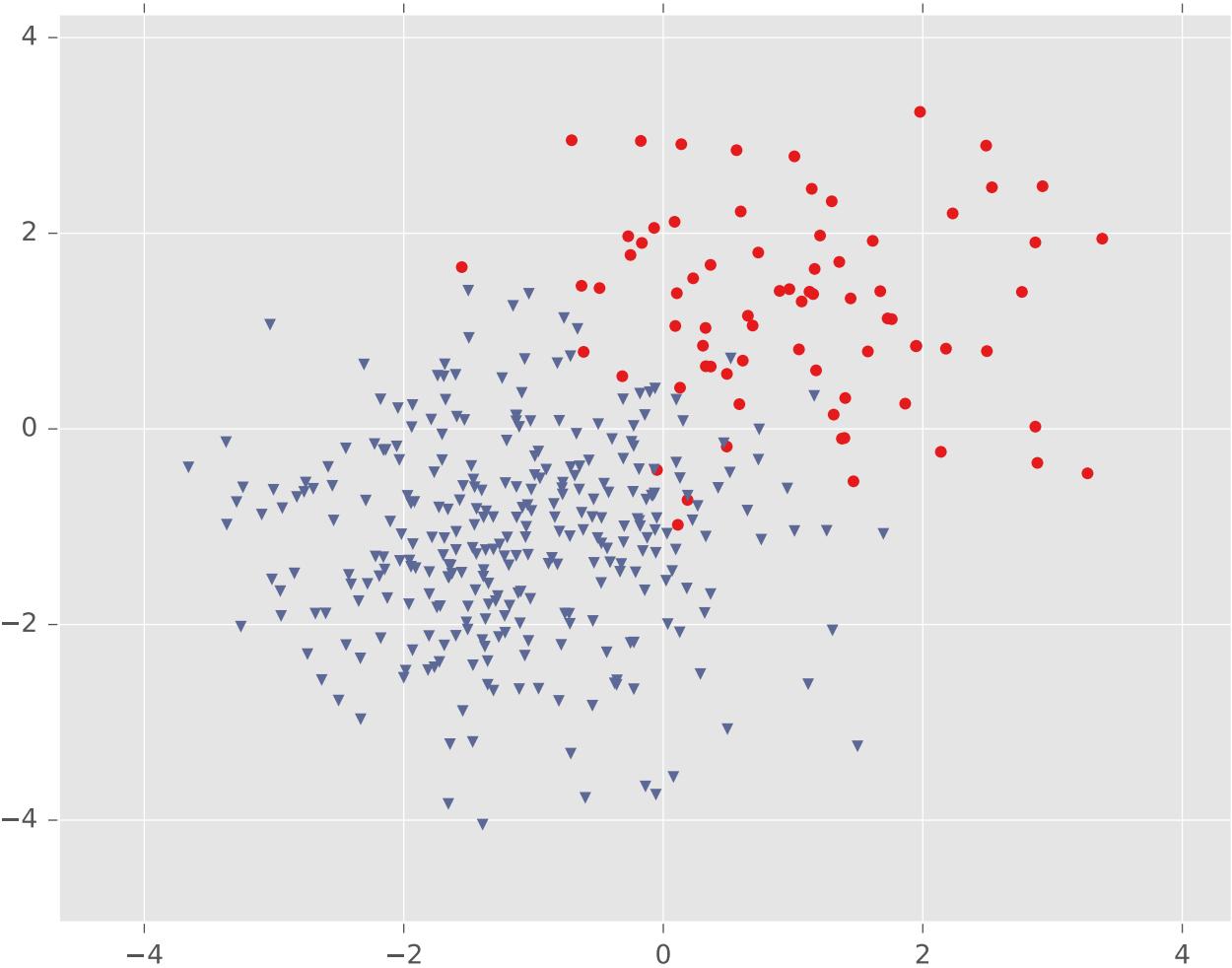
$$\nabla J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N \nabla J^{(i)}$$

- Predictions

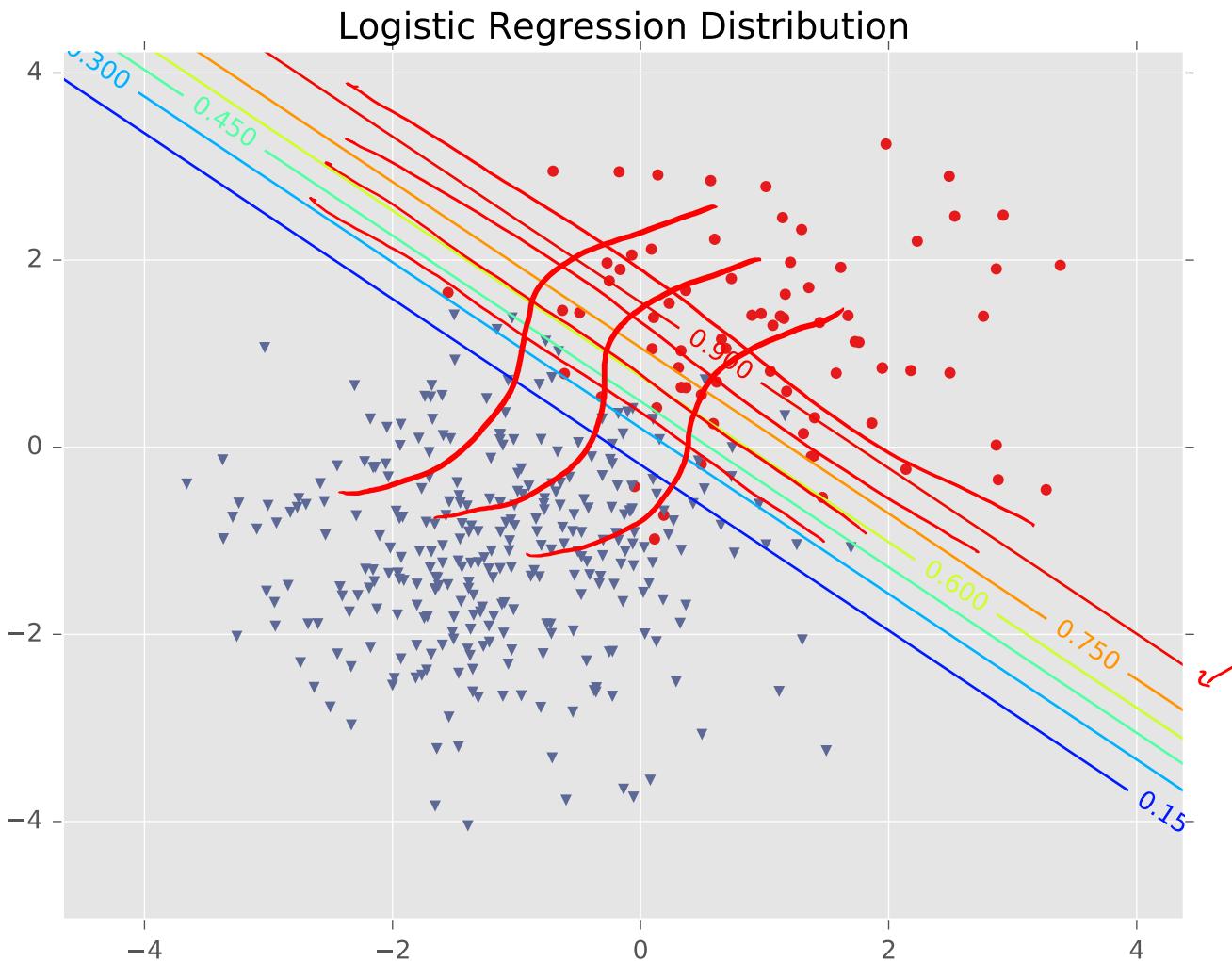
$$\hat{y} = \underset{y \in \{0,1\}}{\operatorname{argmax}} p(y|\mathbf{x}', \widehat{\boldsymbol{\theta}})$$

$$\begin{aligned} &\vdots \\ &= \text{"sign"}(\widehat{\boldsymbol{\theta}}^T \mathbf{x}') \end{aligned}$$

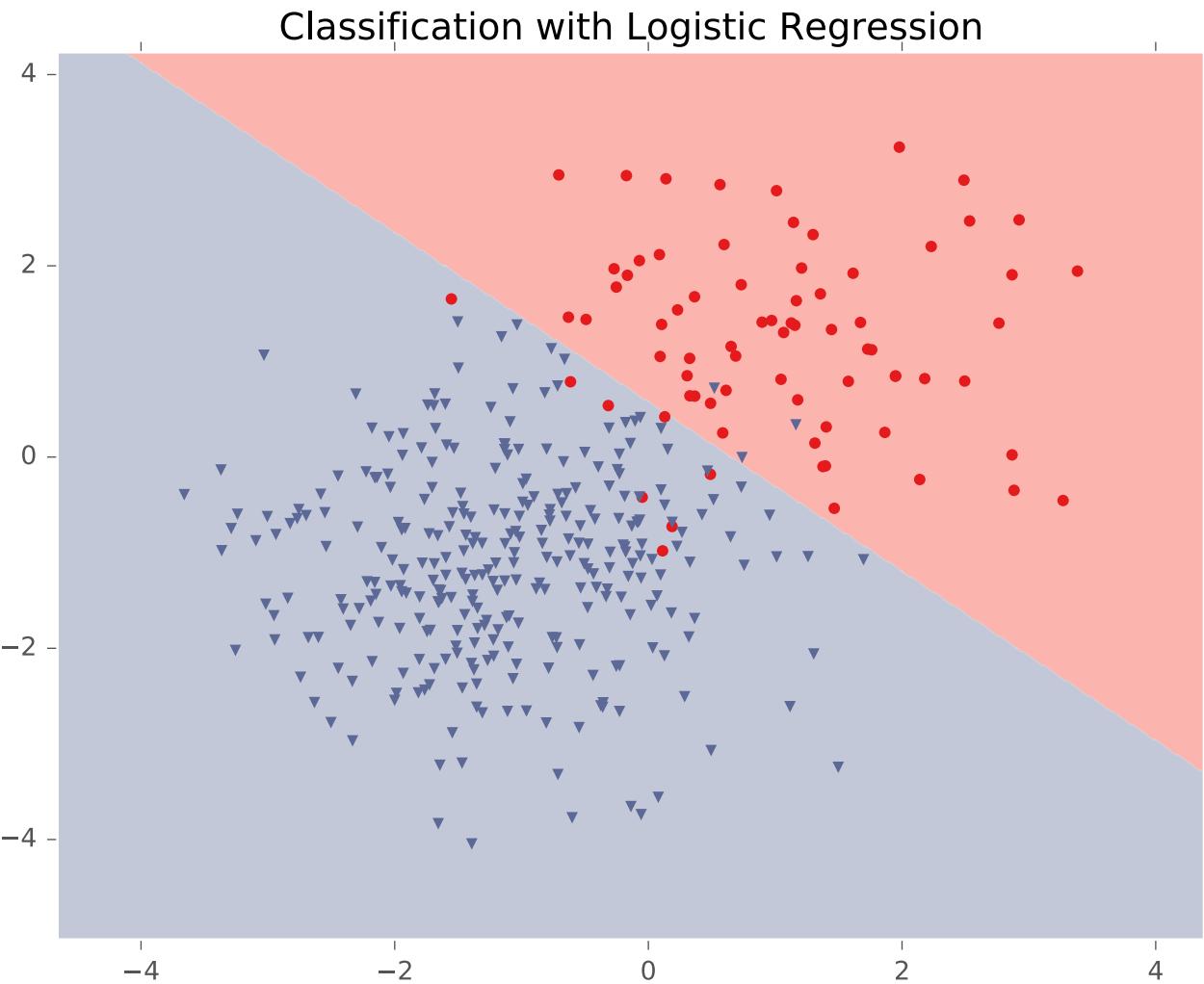
Logistic Regression Decision Boundary



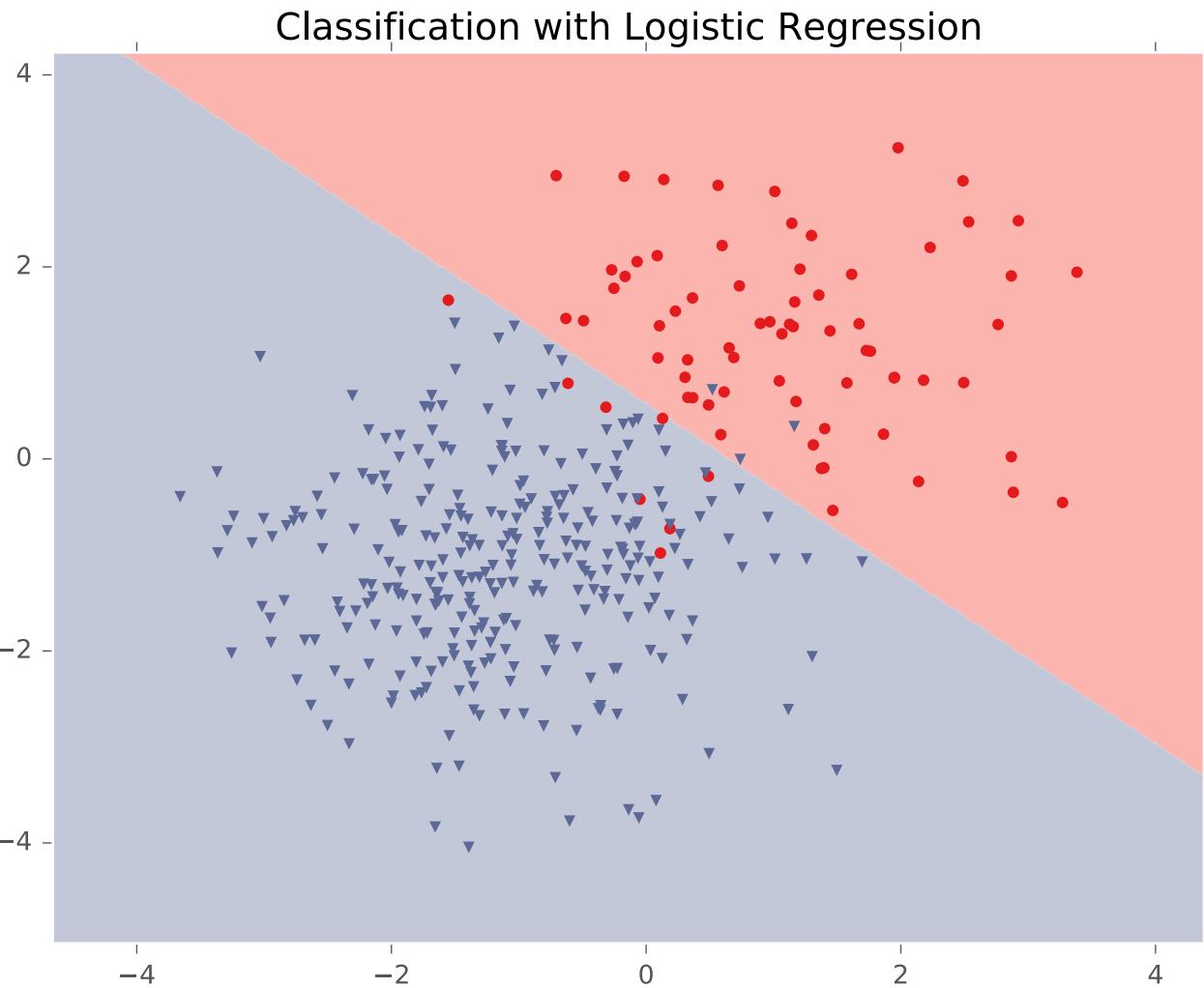
Logistic Regression Decision Boundary



Logistic Regression Decision Boundary



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



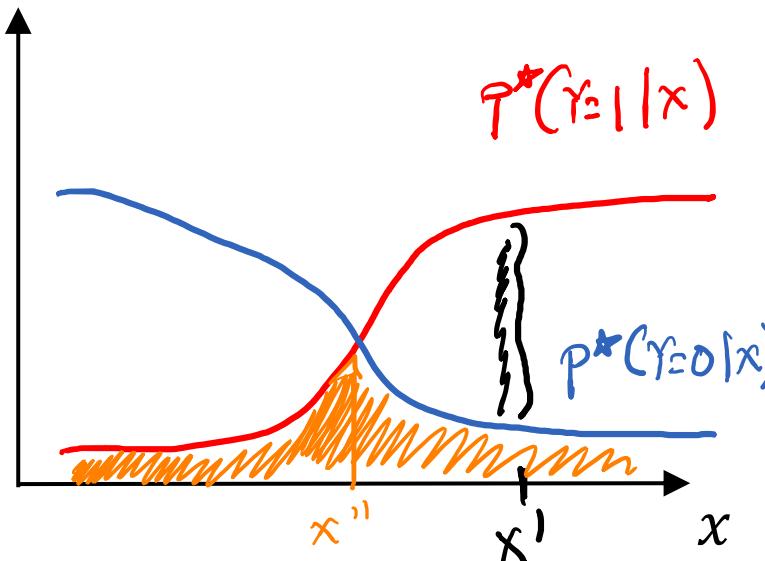
Bayes Optimal Classifier

- Suppose you knew $p^*(Y = 1|x)$ for all x and wanted to minimize the 0-1 loss

$$\ell(\hat{y}, y) = \mathbb{1}(\hat{y} \neq y)$$

- Then the optimal classifier in this setting, called the *Bayes optimal classifier*, is

$$\hat{y} = \begin{cases} 1 & \text{if } p^*(Y = 1|x) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$



- 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^*

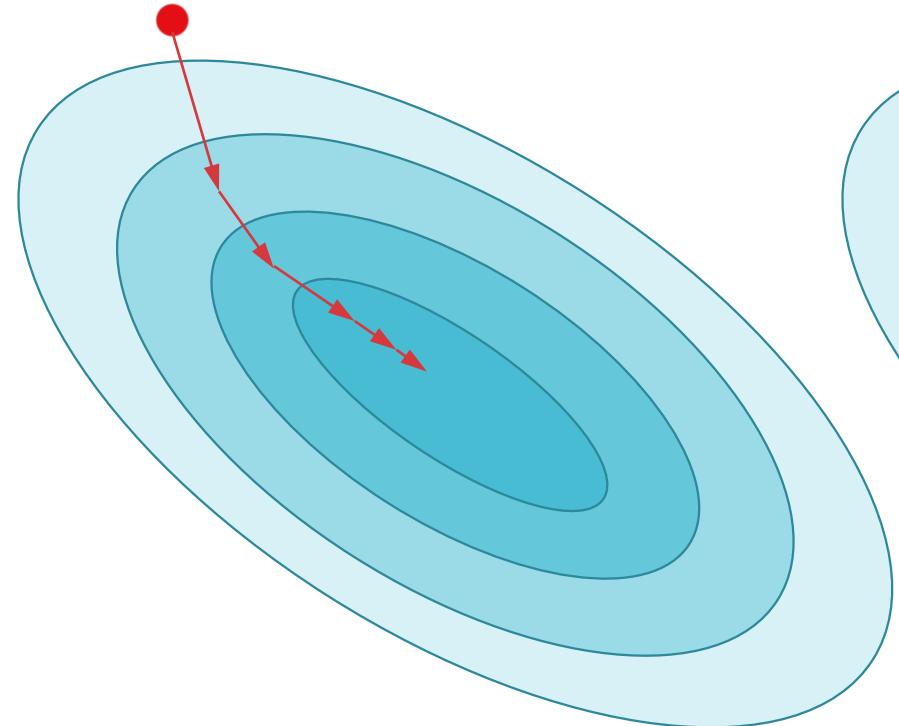
Stochastic Gradient Descent (SGD) for Logistic Regression

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ
- 1. Initialize $\boldsymbol{\theta}^{(0)}$ 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:
$$\nabla J^{(i)}(\boldsymbol{\theta}^{(t)}) = -\underbrace{\left(y^{(i)} - \sigma(\boldsymbol{\theta}^T \mathbf{x}^{(i)})\right)}_{\text{red bracket}} \mathbf{x}^{(i)}$$
 - ii. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla J^{(i)}(\boldsymbol{\theta}^{(t)})$
 - iii. Increment t : $t \leftarrow t + 1$
 - Output: $\boldsymbol{\theta}^{(t)}$

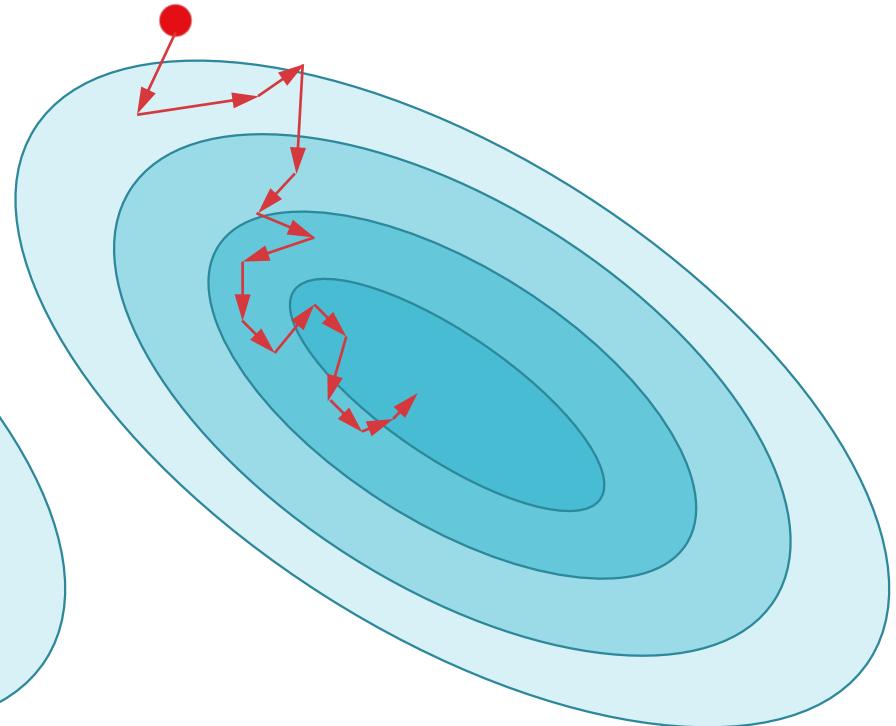
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- 2. While TERMINATION CRITERION is not satisfied
 - a. For $i \in \text{shuffle}(\{1, \dots, N\})$
 - i. Compute the pointwise gradient:
$$\nabla J^{(i)}(\boldsymbol{\theta}^{(t)}) = (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)}) \mathbf{x}^{(i)}$$
 - ii. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla J^{(i)}(\boldsymbol{\theta}^{(t)})$
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Stochastic Gradient Descent vs. Gradient Descent

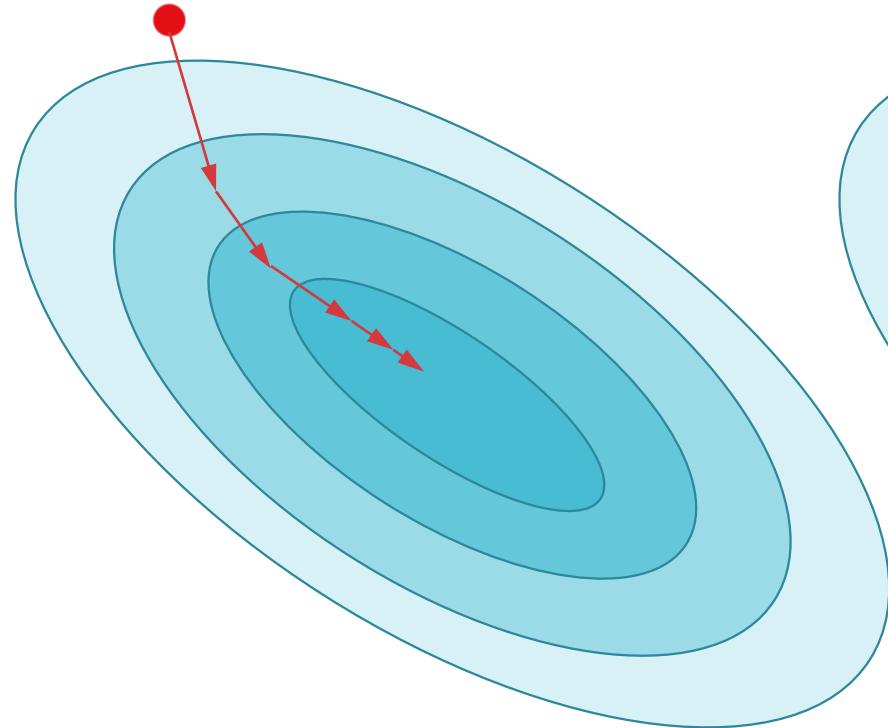


Gradient Descent

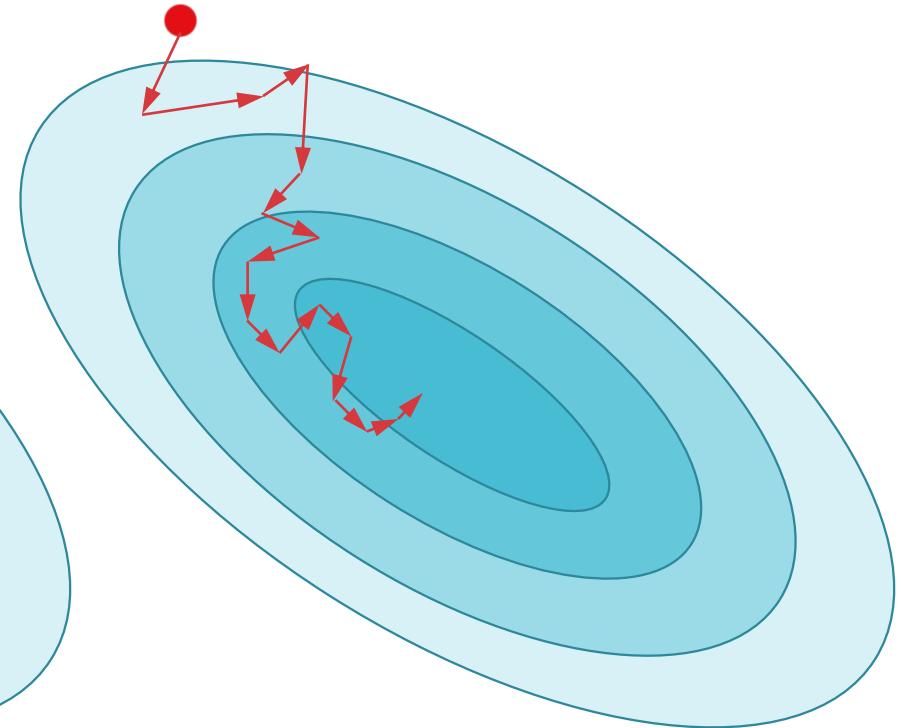


Stochastic Gradient Descent

Can we find
some middle
ground here?



Gradient Descent



Stochastic Gradient Descent

Mini-batch Stochastic Gradient Descent for Neural Networks

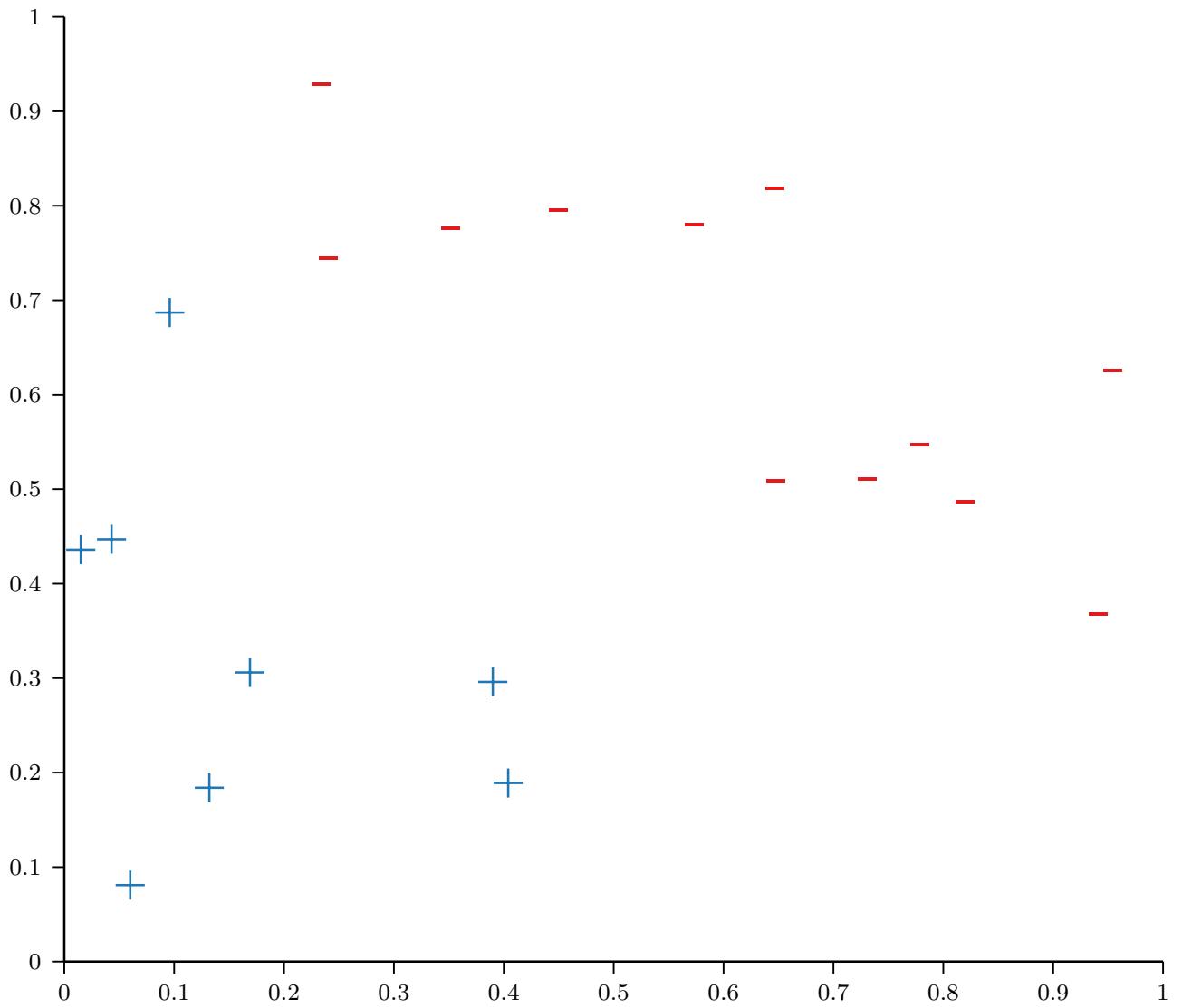
- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$, step size γ , and batch size B
- 1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
- 2. While TERMINATION CRITERION is not satisfied
 - a. Randomly sample B data points from \mathcal{D} , $\{(\mathbf{x}^{(b)}, y^{(b)})\}_{b=1}^B$
 - 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

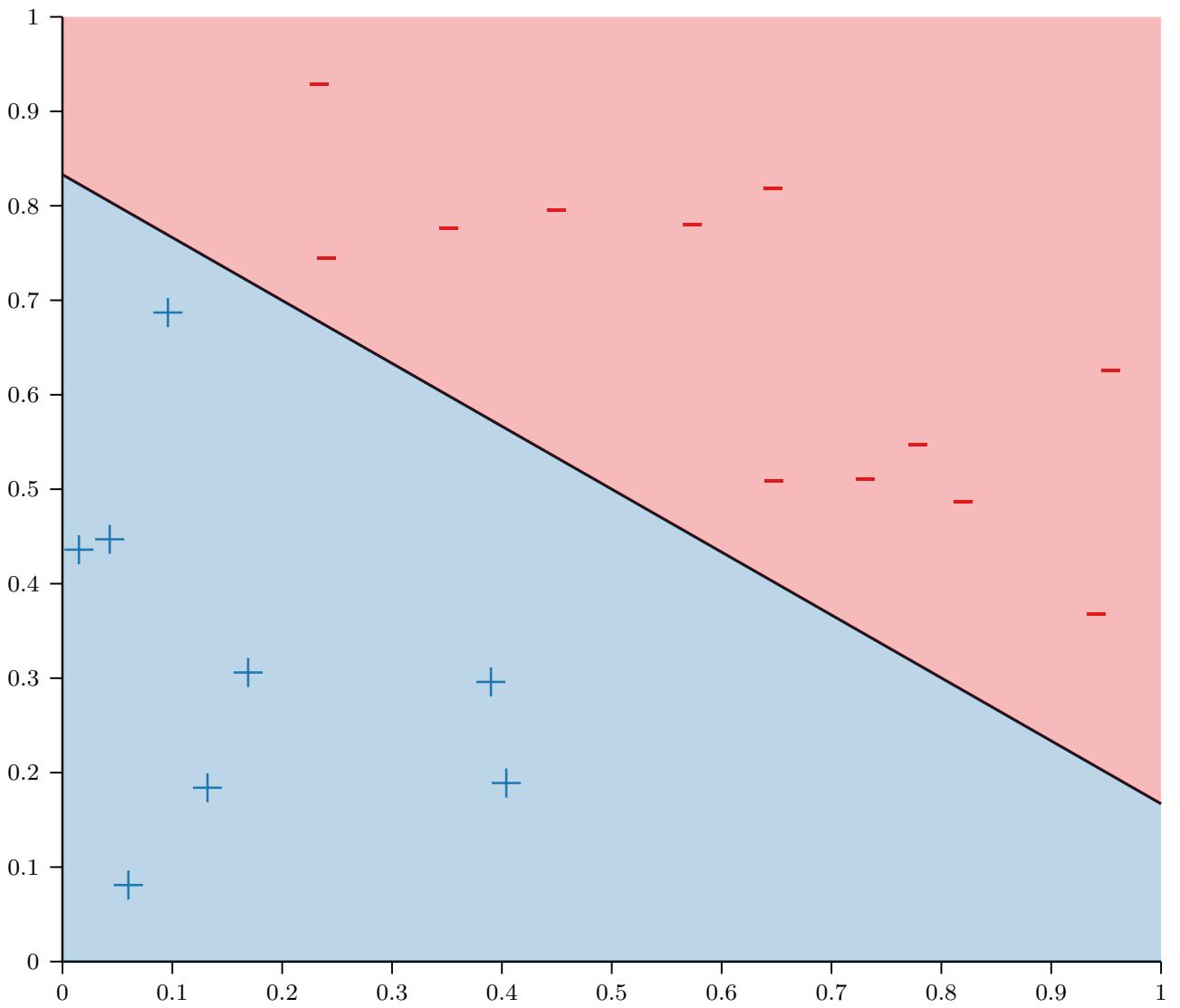
You should be able to...

- 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

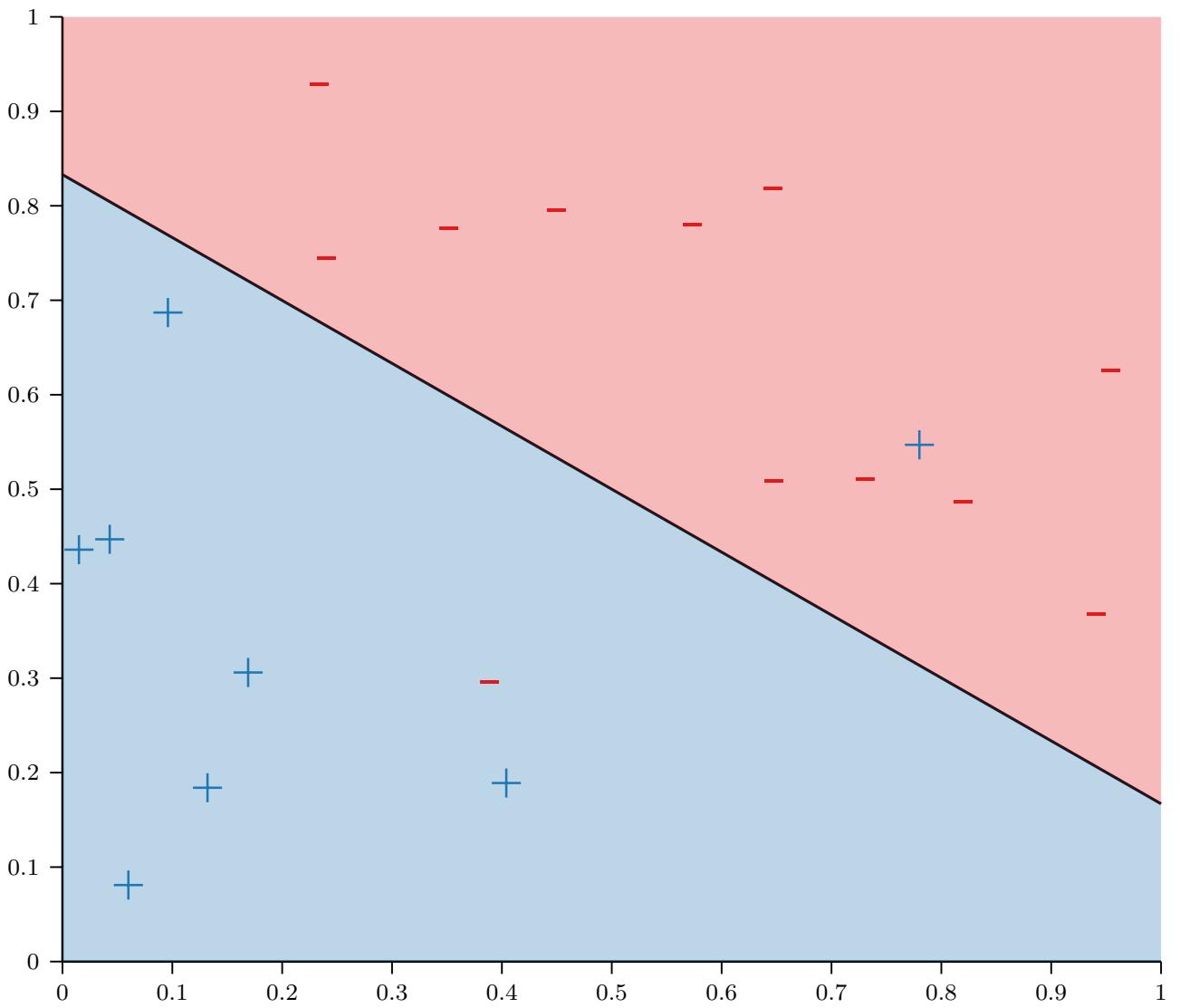
Linear Models



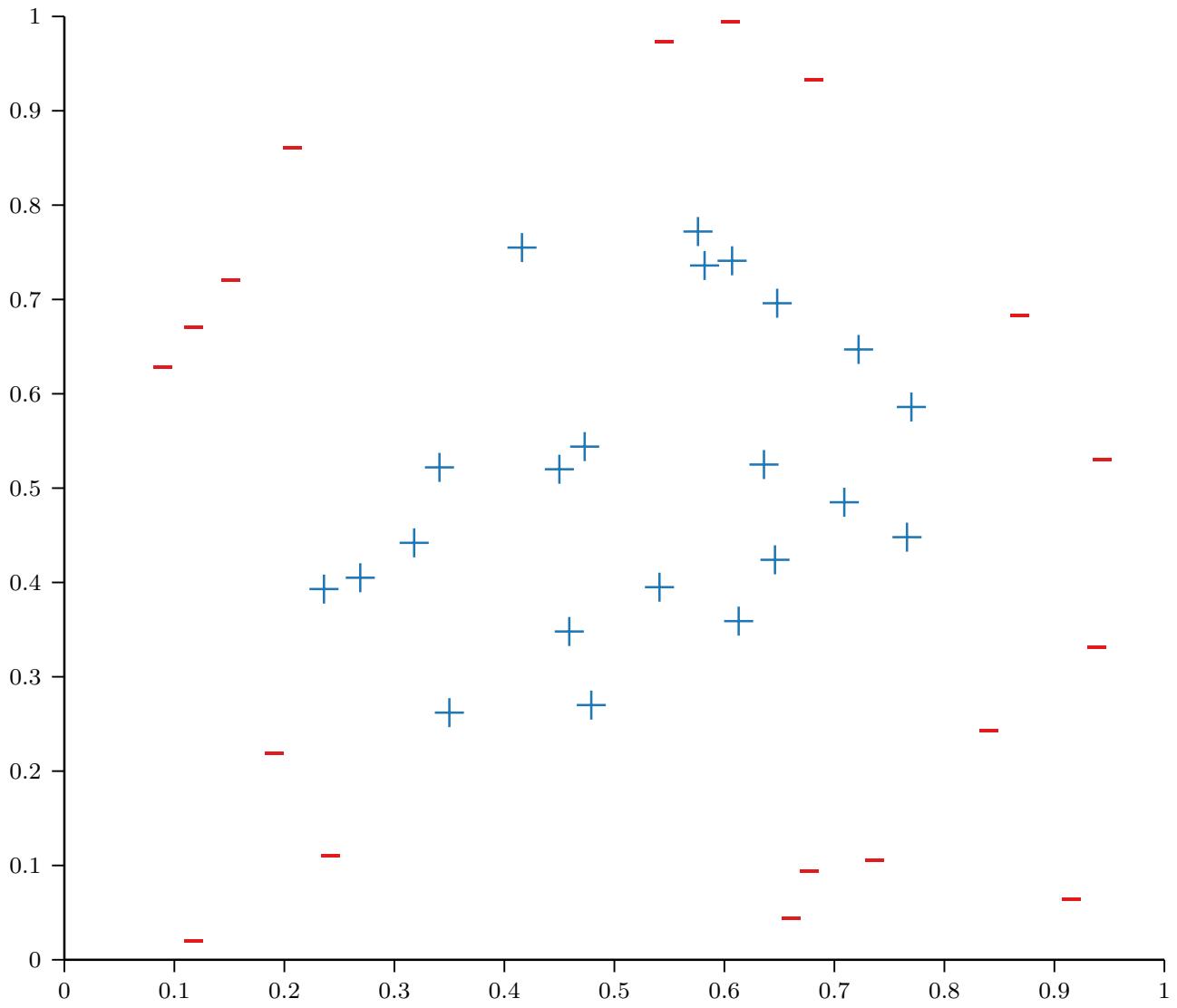
Linear Models



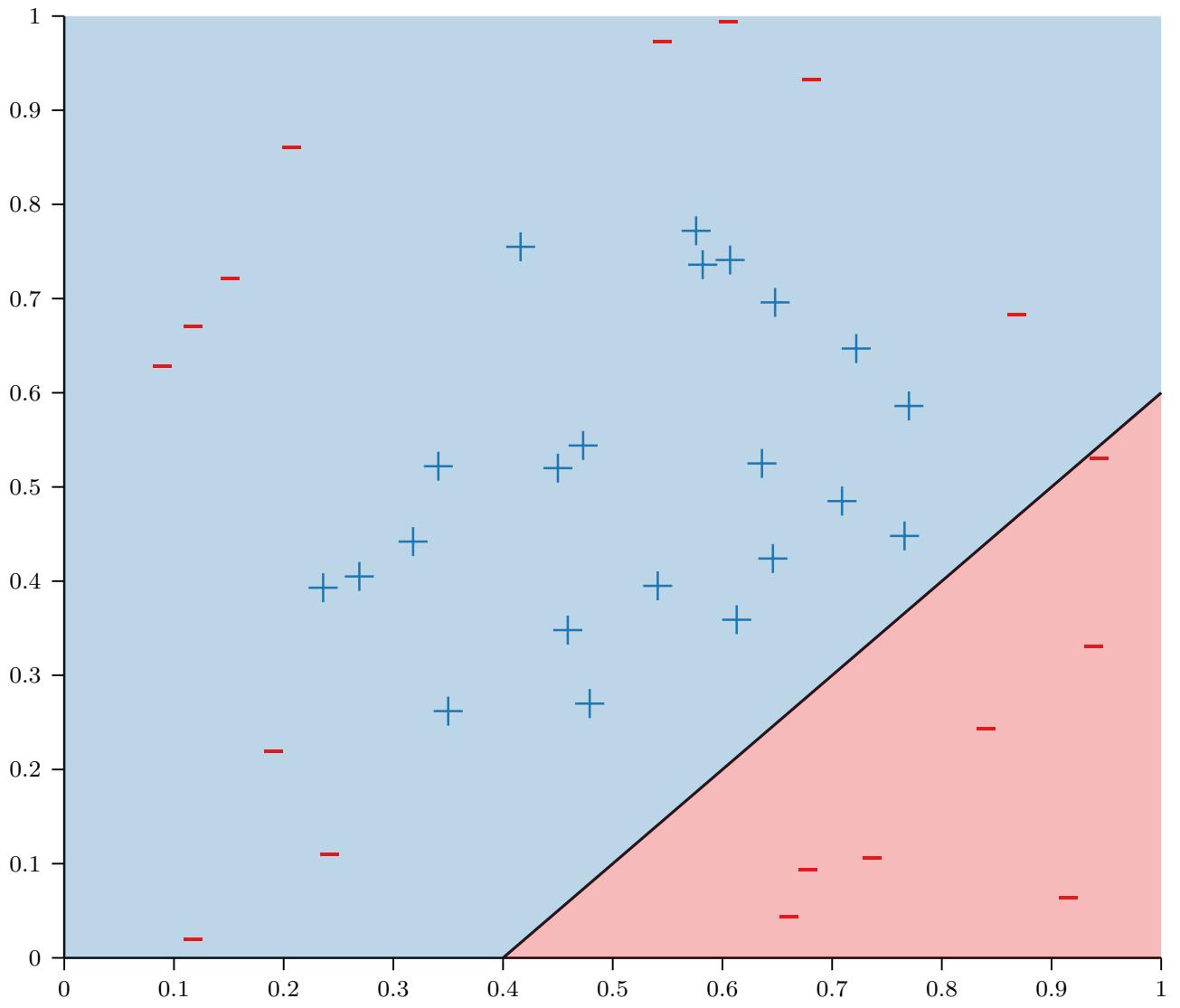
Linear Models



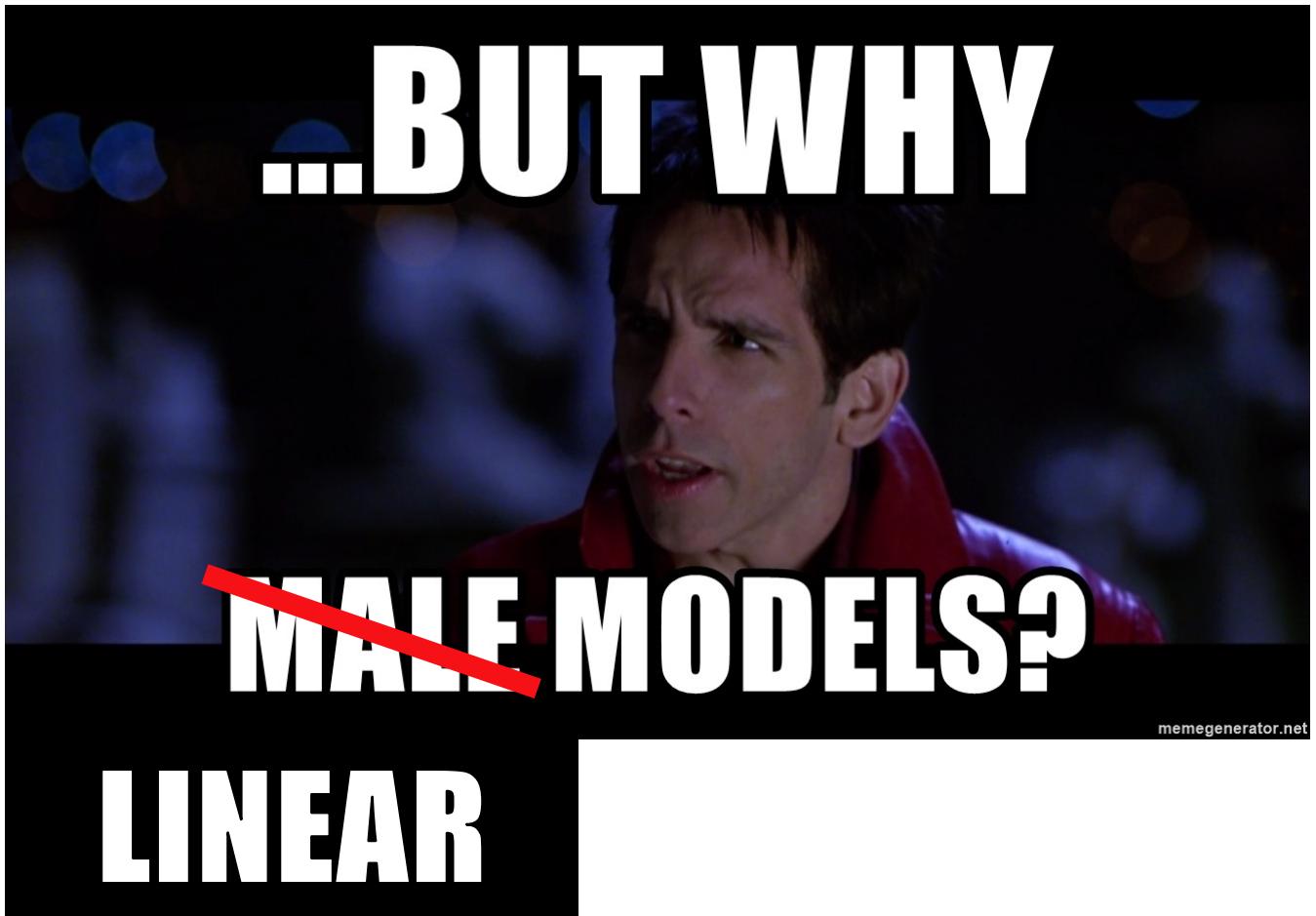
Linear Models?



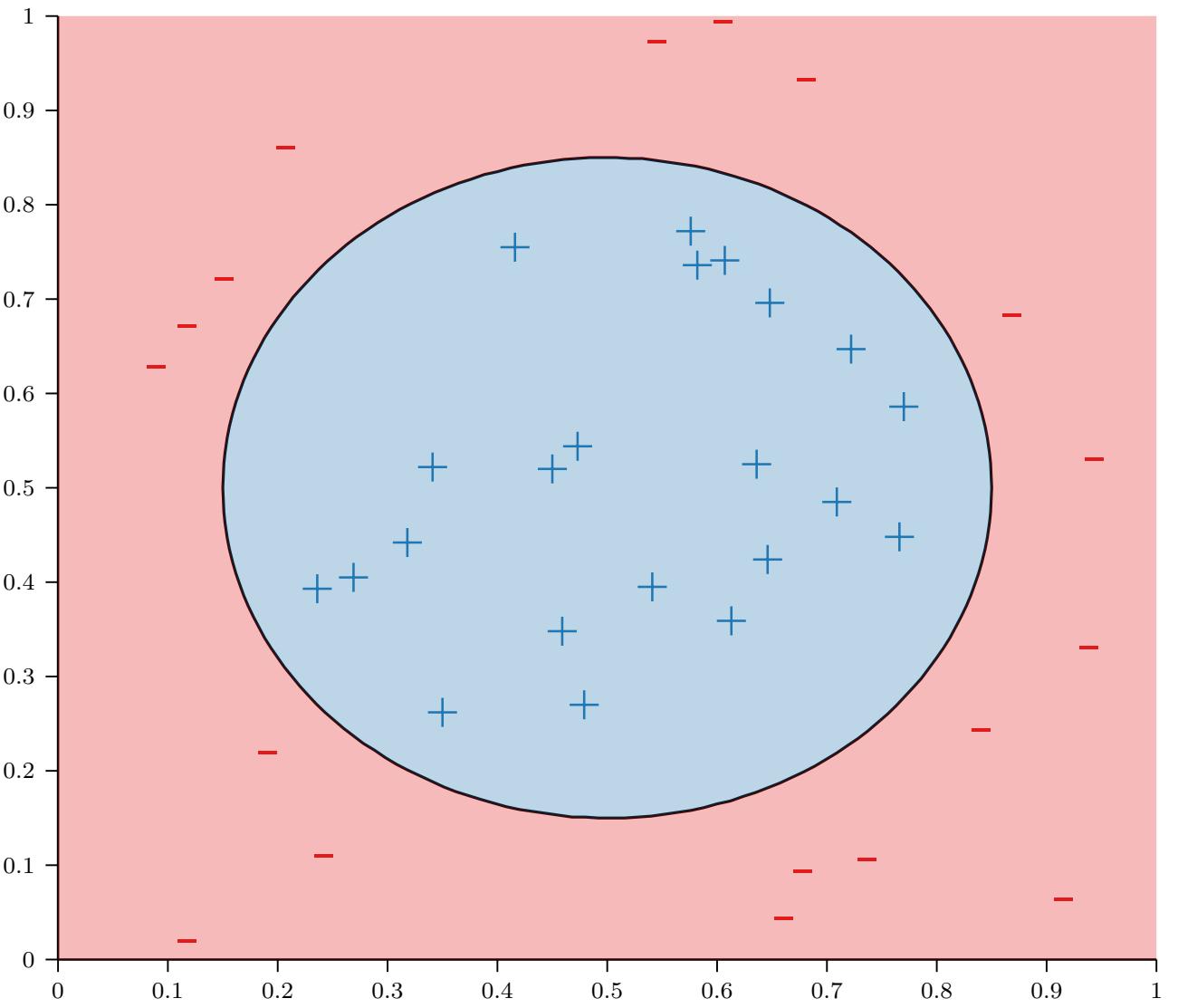
Linear Models?



Linear Models?



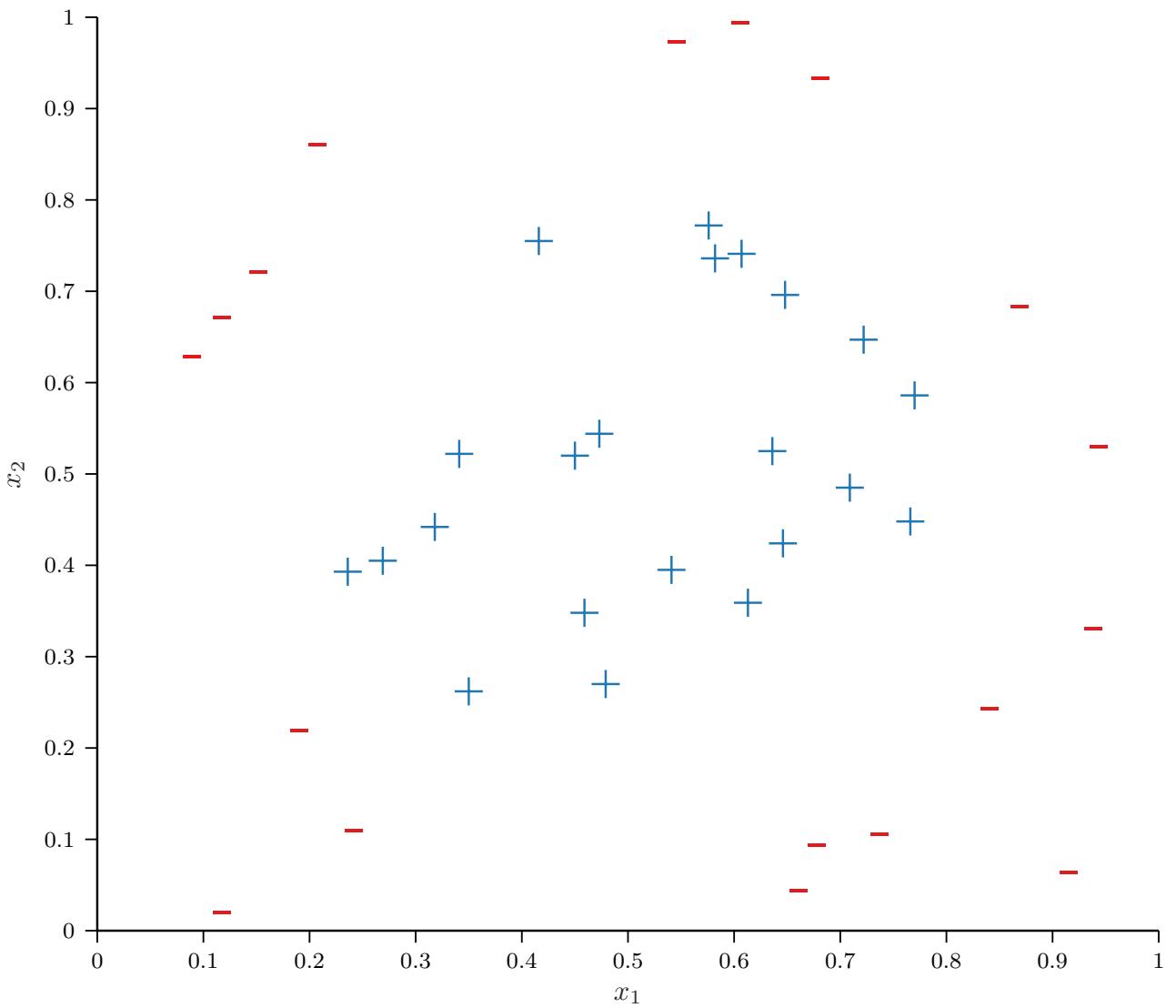
Nonlinear Models



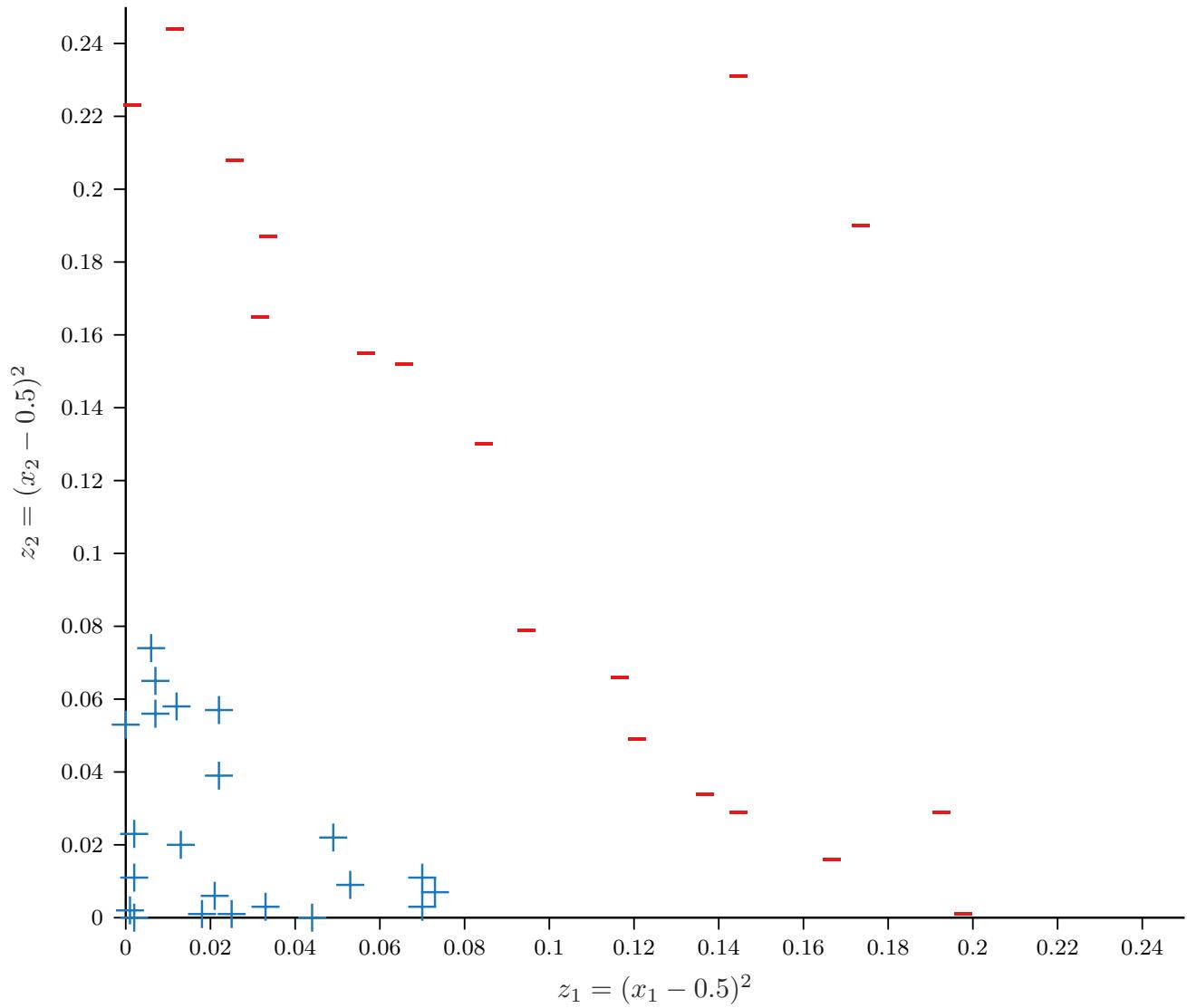
Feature Transforms

- Given D -dimensional inputs $\mathbf{x} = [x_1, \dots, x_D]$, first compute some transformation of our input, e.g.,
$$\phi([x_1, x_2]) = [z_1 = (x_1 - 0.5)^2, z_2 = (x_2 - 0.5)^2]$$

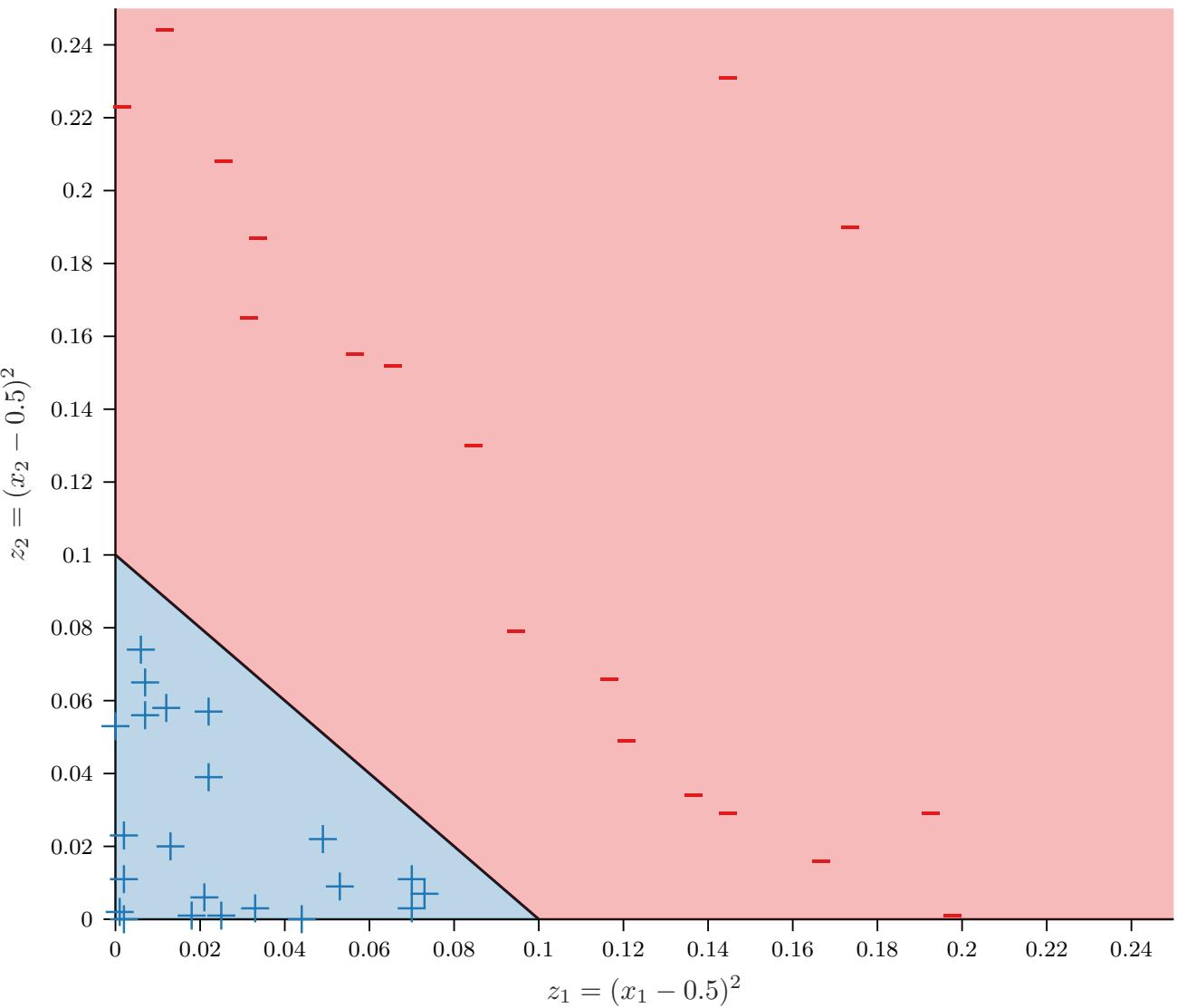
Nonlinear Models



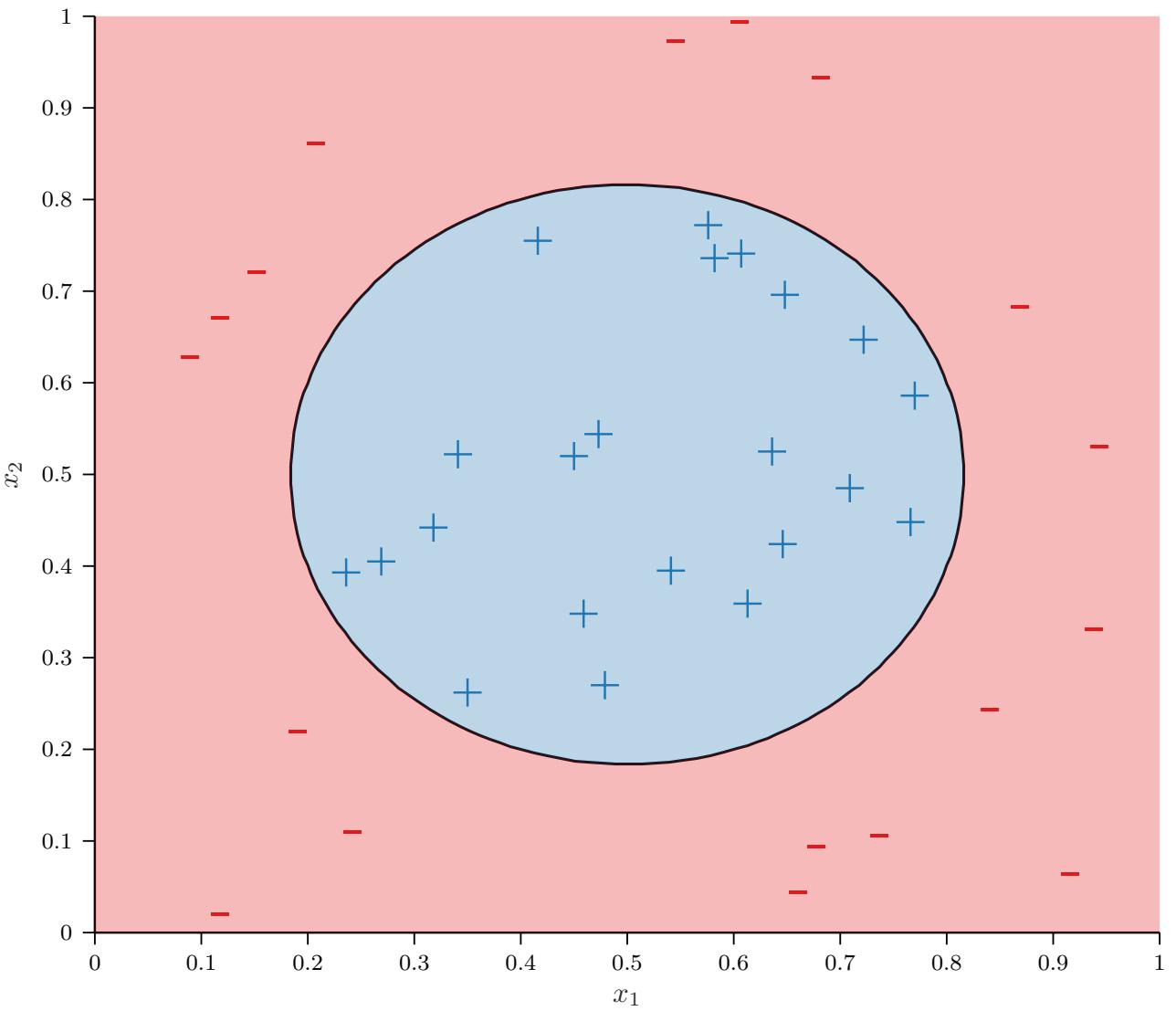
Nonlinear Models



Nonlinear Models



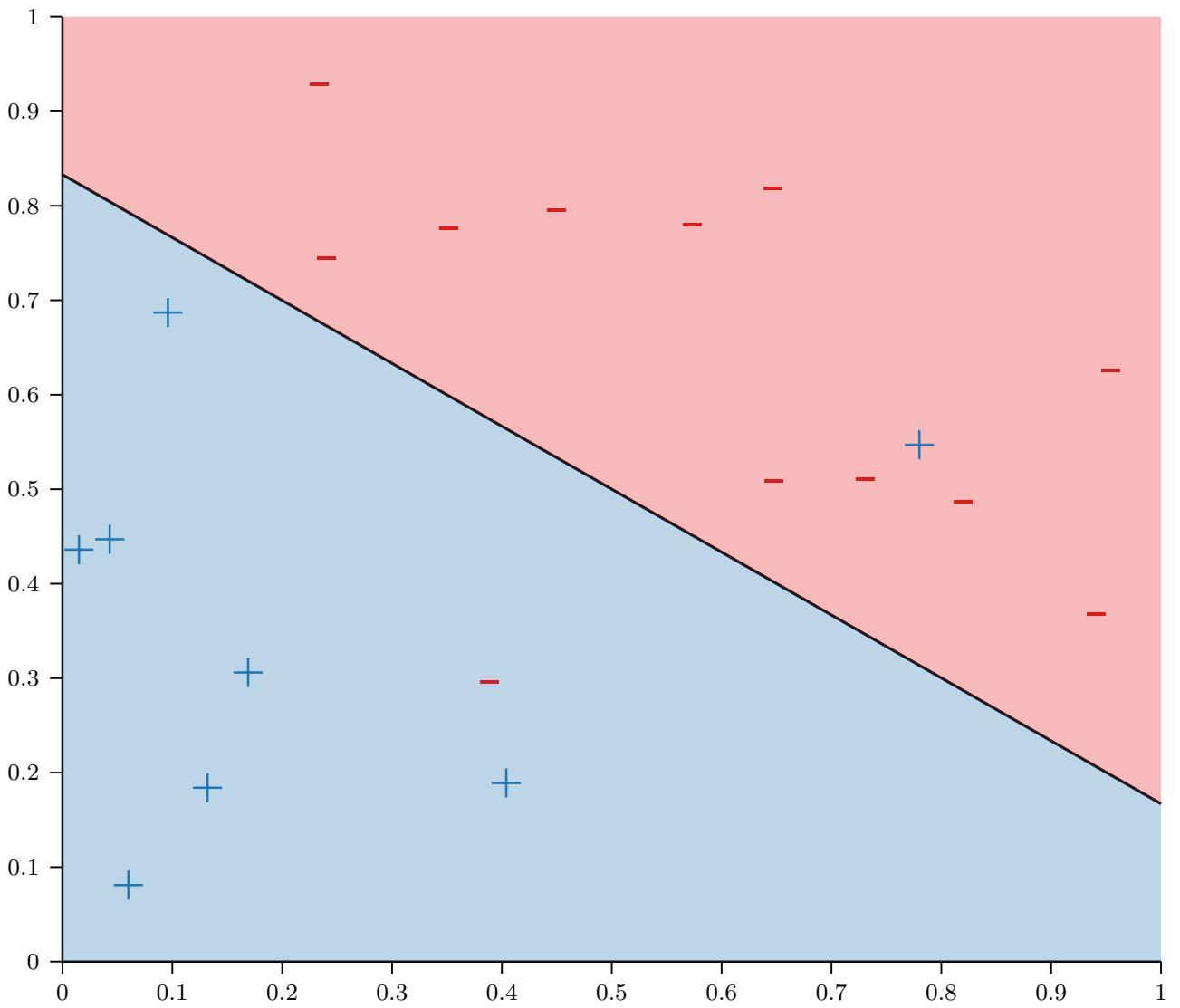
Nonlinear Models



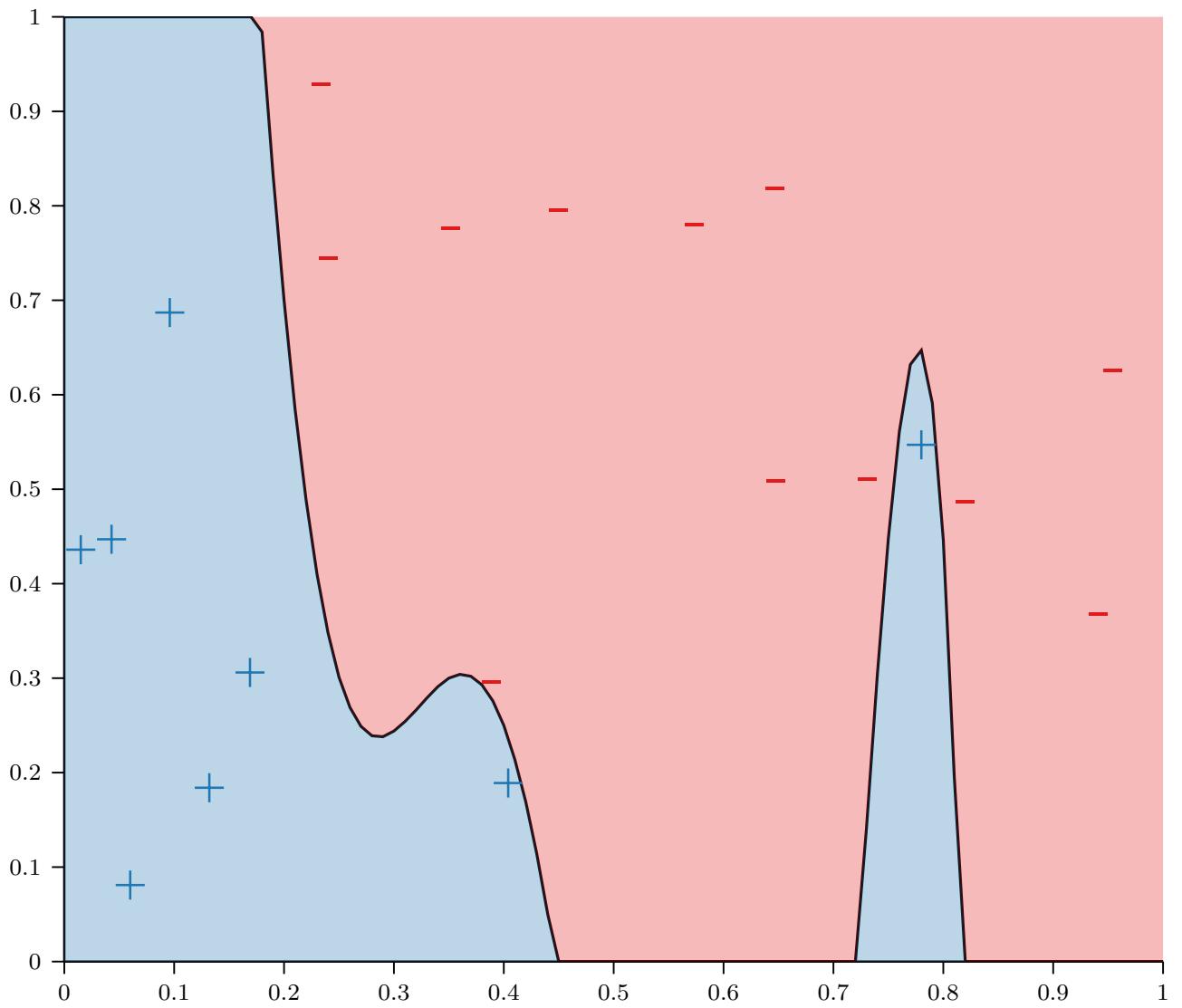
General Q^{th} -order Transforms

- input size polynomial order
- $\phi_{2,2}([x_1, x_2]) = [x_1, x_2, x_1^2, x_1 x_2, x_2^2]$
 - $\phi_{2,3}([x_1, x_2]) = [x_1, x_2, x_1^2, x_1 x_2, x_2^2, x_1^3, x_1^2 x_2, x_1 x_2^2, x_2^3]$
 - $\phi_{2,4}([x_1, x_2]) = [x_1, x_2, x_1^2, x_1 x_2, x_2^2, x_1^3, x_1^2 x_2, x_1 x_2^2, x_2^3, x_1^4, x_1^3 x_2, x_1^2 x_2^2, x_1 x_2^3, x_2^4]$
 - $\phi_{2,Q}$ 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

	Low-Dimensional Input Space	High-Dimensional Input Space
Training Error	High	Low
Generalization	Good	Bad

Feature Transforms: Experiment

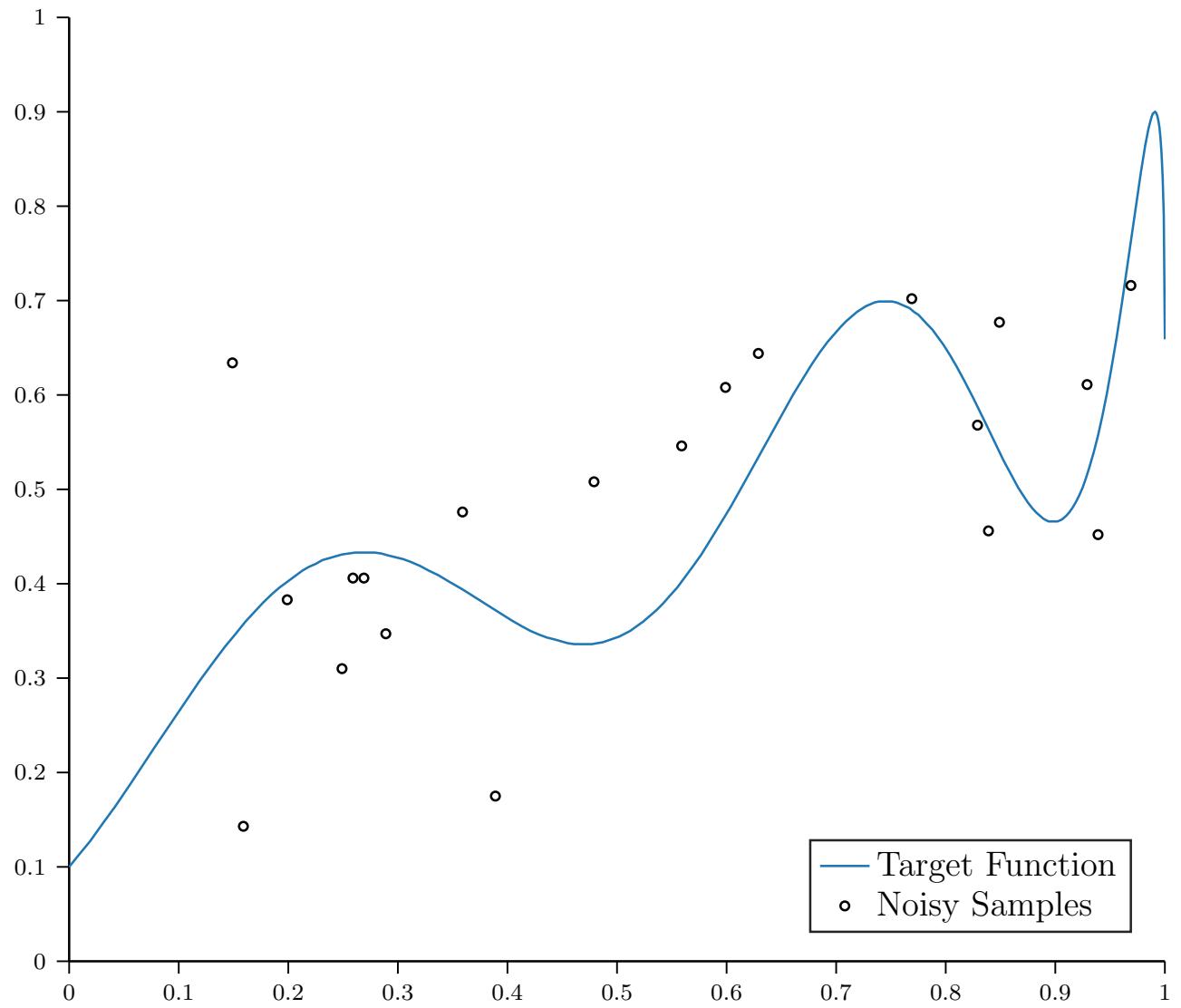
- $x \in \mathbb{R}$, $y \in \mathbb{R}$ and $N = 20$
- Targets are generated by a 10th-order polynomial in x with additive Gaussian noise:

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

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

Noisy Targets

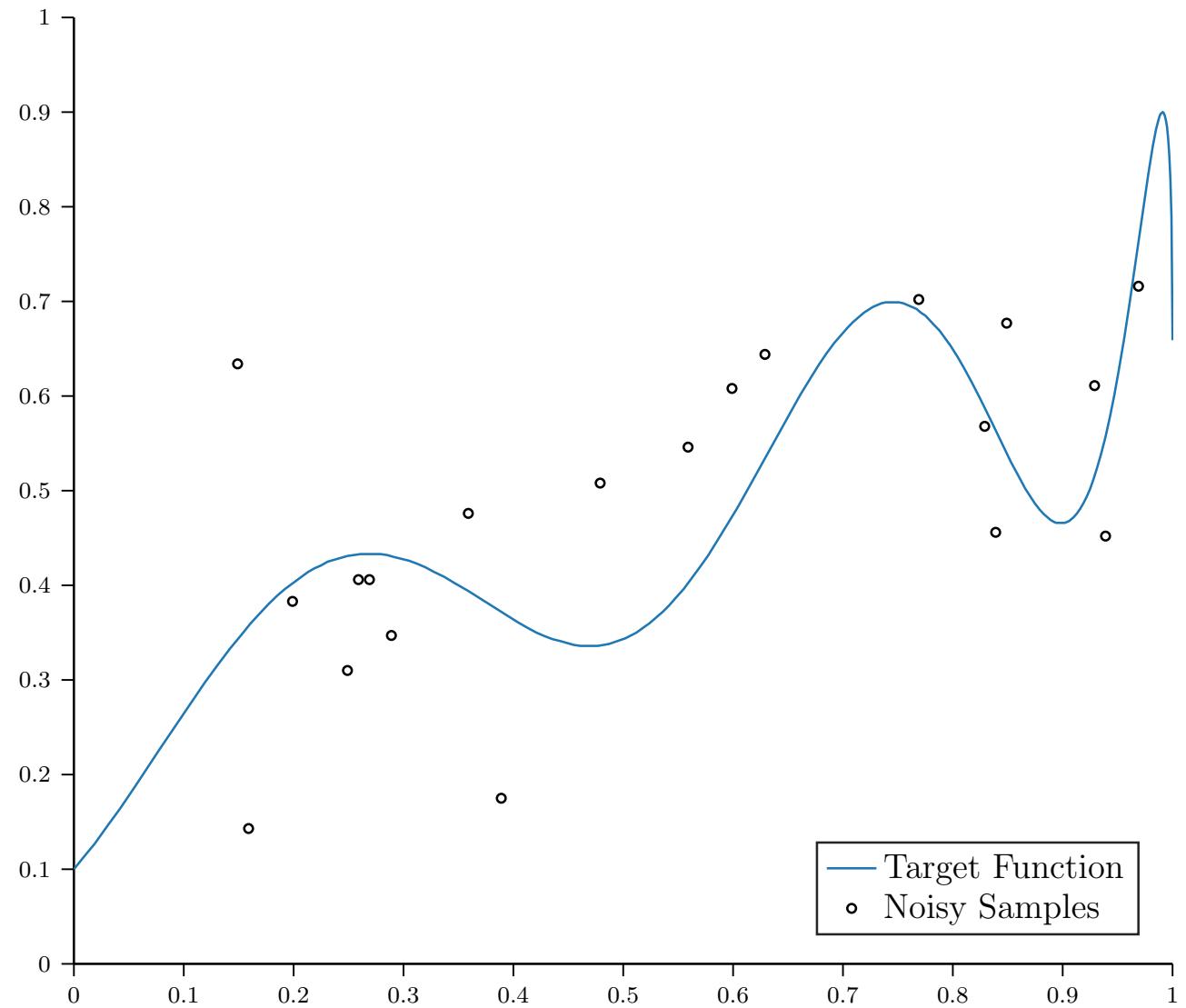
- 10-dimensional target function with additive Gaussian noise
- $\mathcal{H}_2 = 2^{\text{nd}}$ -order polynomial
- $\mathcal{H}_{10} = 10^{\text{th}}$ -order polynomial



Poll Question 1

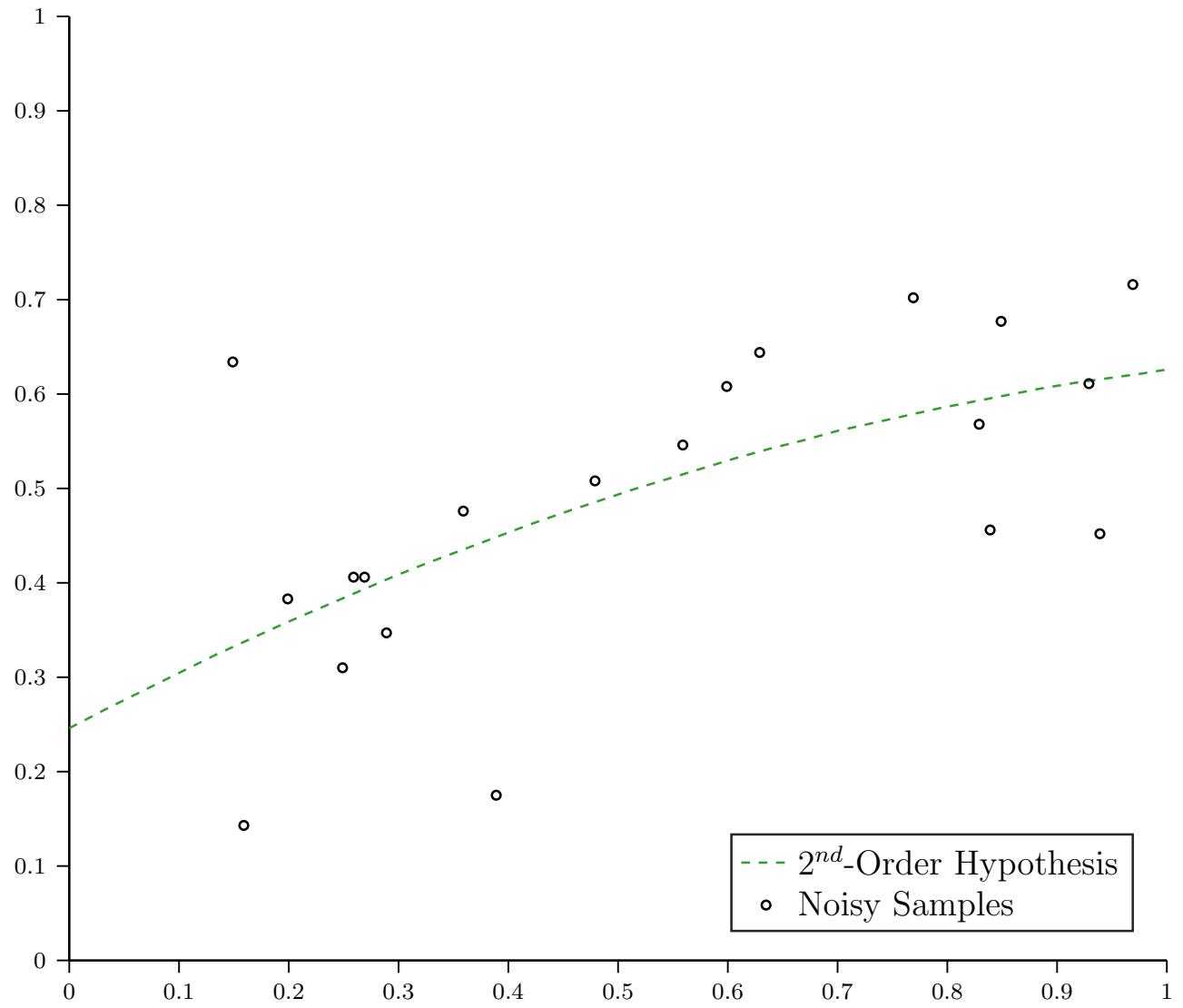
Which model do you think will have a lower true error?

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



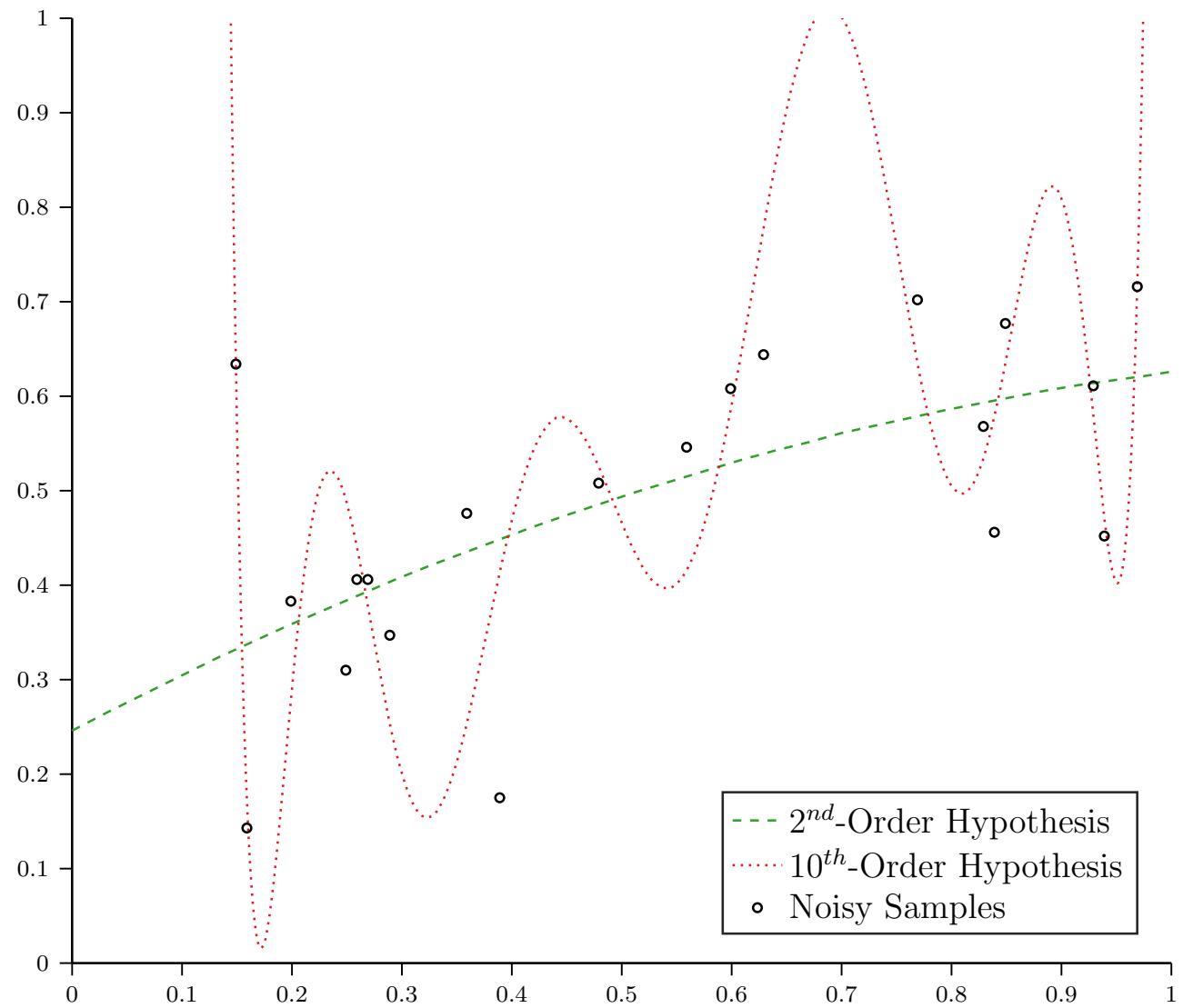
Noisy Targets

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



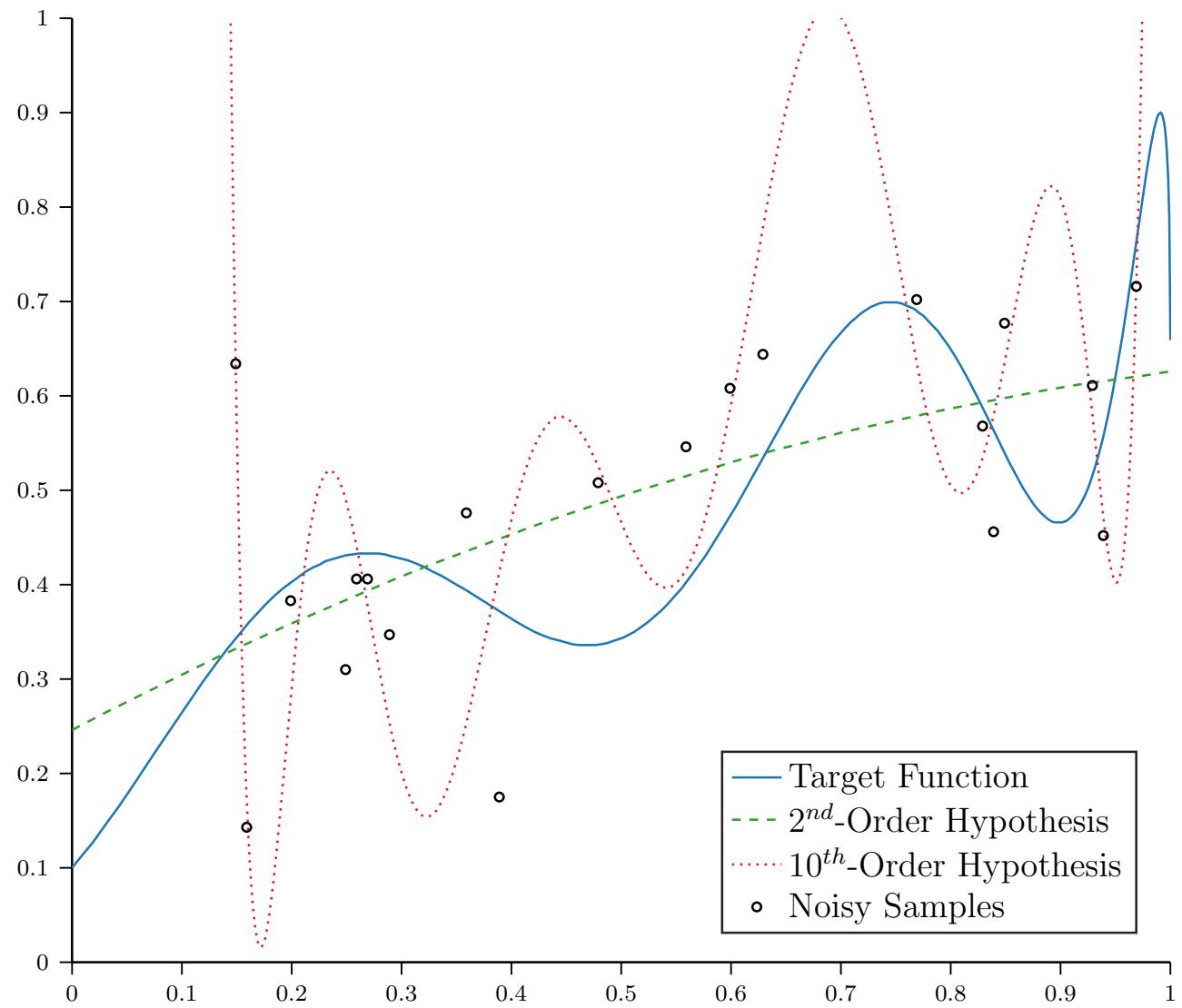
Noisy Targets

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



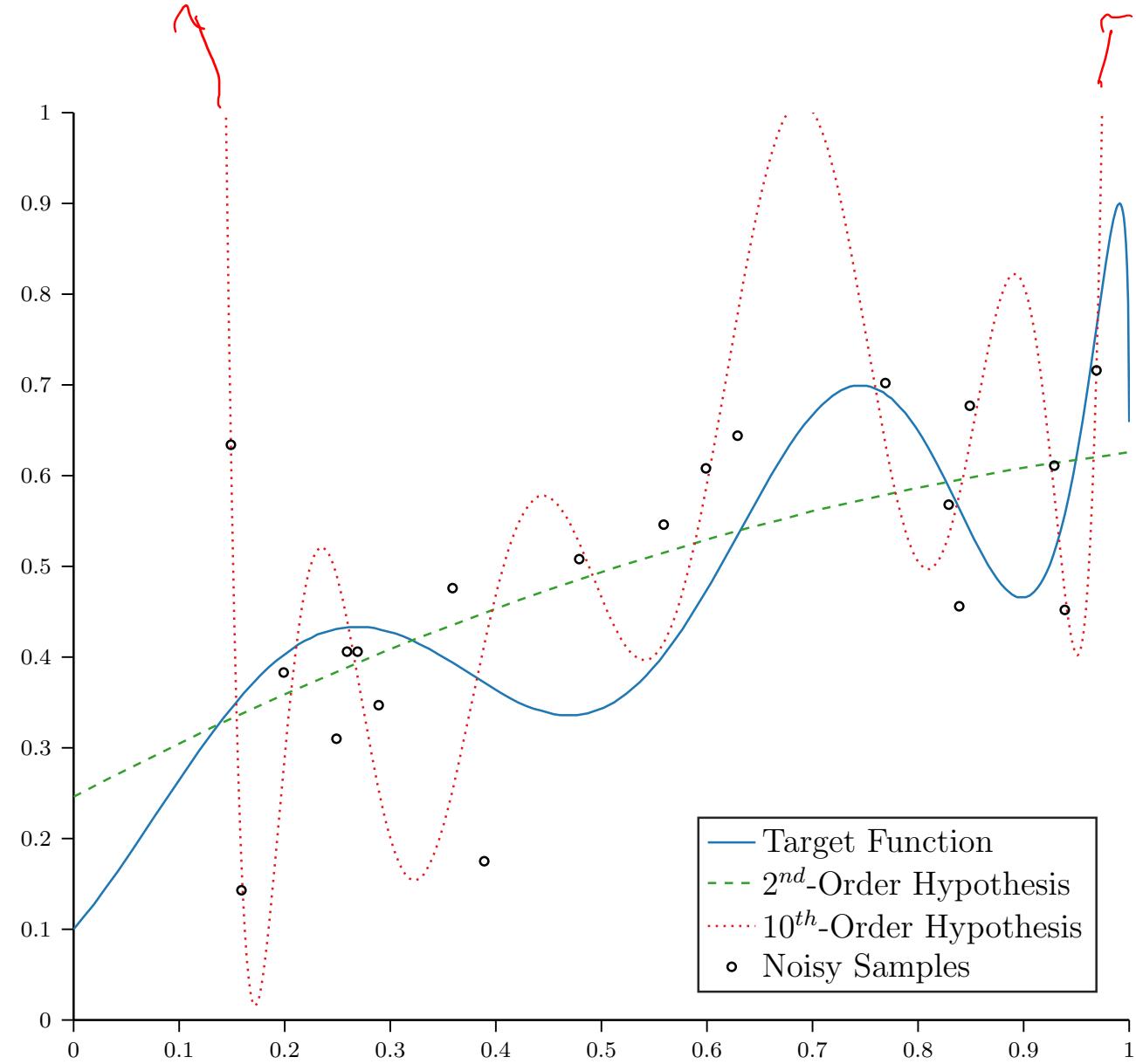
Noisy Targets

- 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 10th-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}

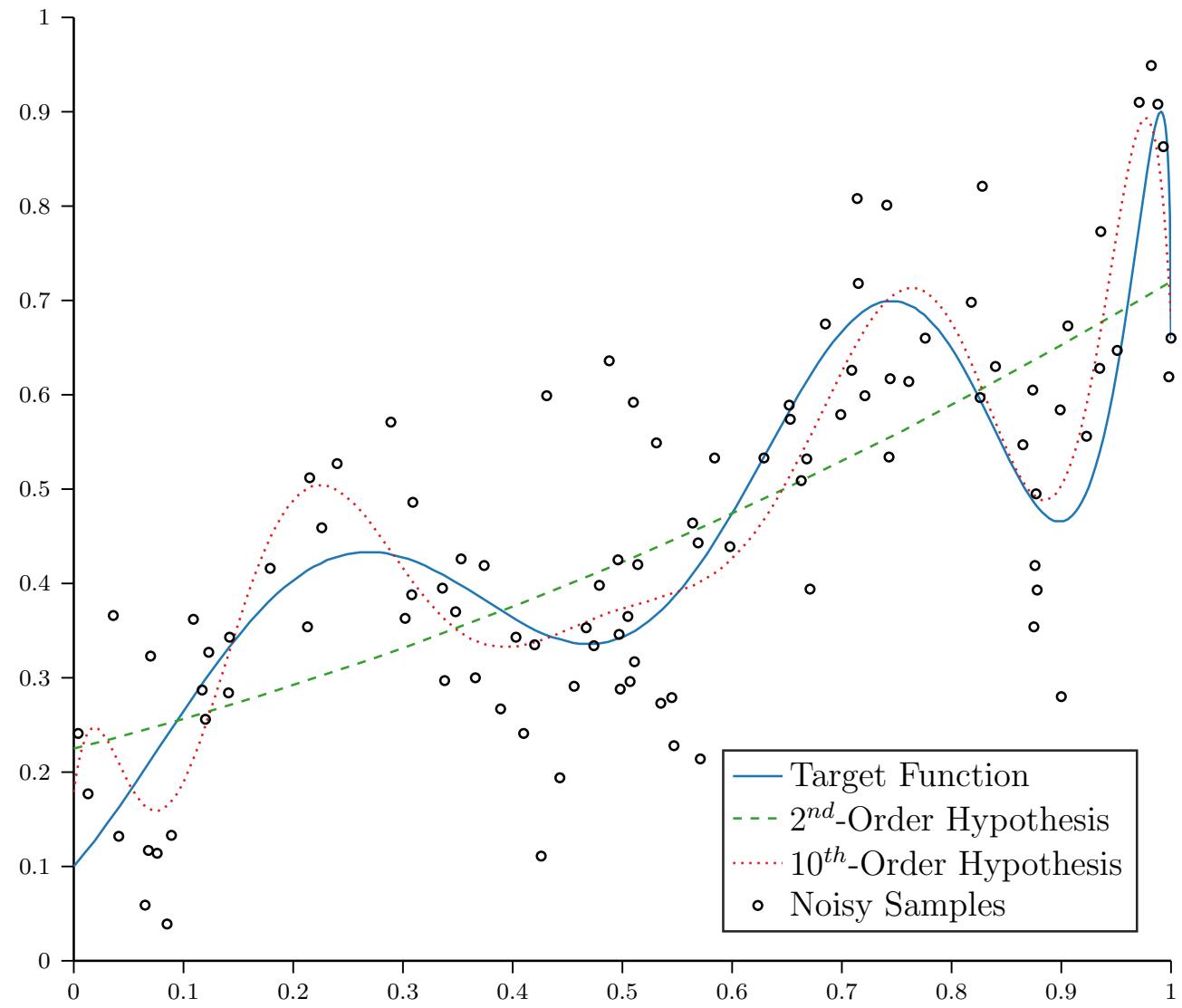
- $x \in \mathbb{R}, y \in \mathbb{R}$ and $N = 100$
- Targets are generated by a 10th-order polynomial in x with additive Gaussian noise:

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

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

- $\mathcal{H}_{10} = 10^{\text{th}}$ -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 $(X\theta - y)^T(X\theta - y)$
- 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, ϕ 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 $\boldsymbol{\omega}$ that minimizes

$$(X\boldsymbol{\theta} - \mathbf{y})^T(X\boldsymbol{\theta} - \mathbf{y})$$

- Subject to:

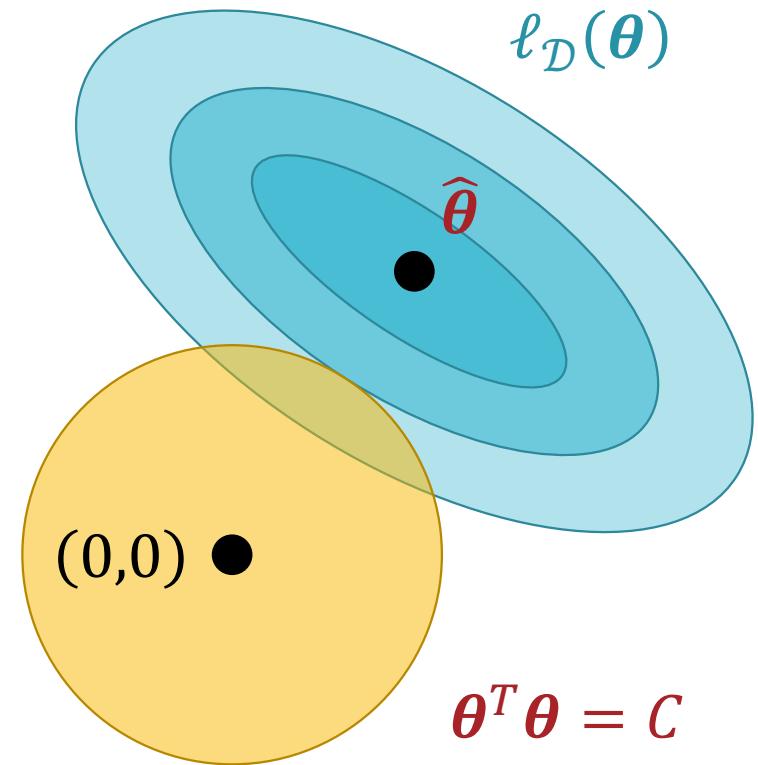
$$\|\boldsymbol{\theta}\|_2^2 = \boldsymbol{\theta}^T \boldsymbol{\theta} = \sum_{d=0}^D \theta_d^2 \leq C$$

Soft Constraints

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

$$(\boldsymbol{\theta}_0^T + \boldsymbol{\theta}_1^T) \leq C$$

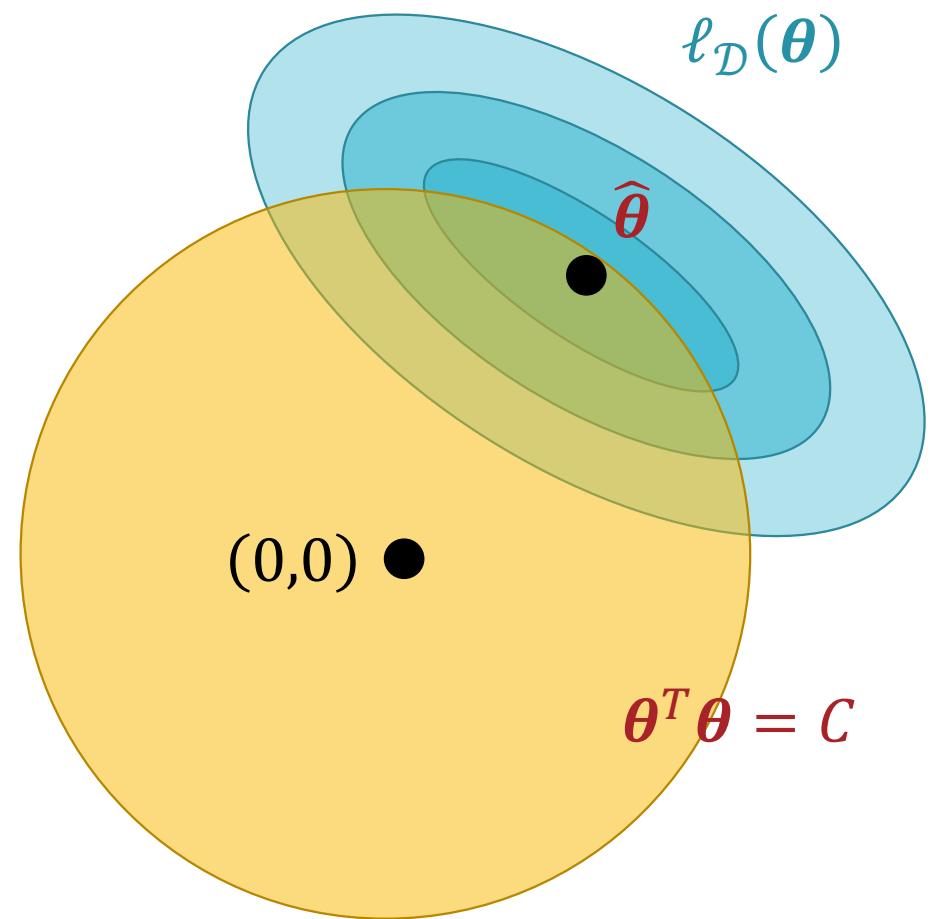
$$\text{subject to } \boldsymbol{\theta}^T \boldsymbol{\theta} \leq C$$



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

$$\text{minimize } \ell_D(\theta) = (X\theta - y)^T(X\theta - y)$$

subject to $\theta^T \theta \leq C$ *(proportional to)*

$$\nabla_{\theta} \ell_D(\hat{\theta}_{REG}) \propto -\hat{\theta}_{REG}$$

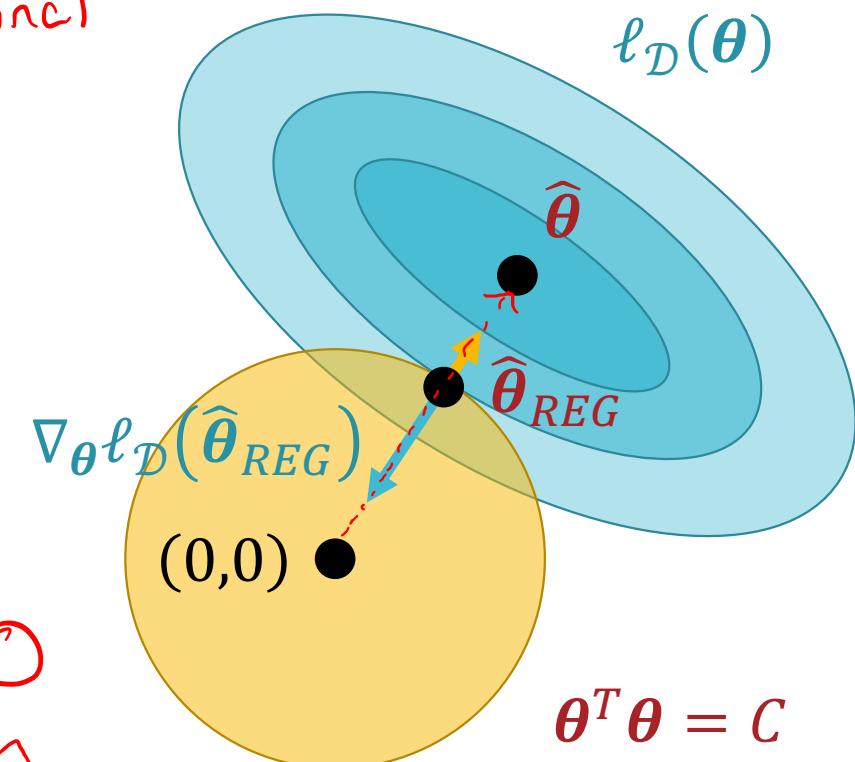
$$\rightarrow \nabla_{\theta} \ell_D(\hat{\theta}_{REG}) = -2\lambda \hat{\theta}_{REG}$$

$$\lambda_c \geq 0$$

$$\Rightarrow \nabla_{\theta} \ell_D(\hat{\theta}_{REG}) + 2\lambda_c \hat{\theta}_{REG} = 0$$

$$\Rightarrow \nabla_{\theta} (\ell_D(\hat{\theta}_{REG}) + \lambda_c \hat{\theta}_{REG}^T \hat{\theta}_{REG}) = 0$$

$$\min \cdot \ell_D(\theta) + \lambda_c \theta^T \theta$$



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

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

$$\text{s.t. } \lambda_C \geq 0$$

Ridge Regression

$$(\lambda_C \geq 0)$$

10/2/23

$$\rightarrow (X^T \theta - y)^T (X^T \theta - y)$$

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

$$\nabla_{\theta} \ell_D^{AUG}(\theta) = 2 X^T X \theta - 2 X^T y + 2 \lambda_C \theta$$

$$\Rightarrow 2 X^T X \hat{\theta}_{REG} - 2 X^T y + 2 \lambda_C \hat{\theta}_{REG} = 0$$

$$\Rightarrow \underbrace{X^T X \hat{\theta}_{REG}}_{+ \lambda_C \hat{\theta}_{REG}} = \underbrace{X^T y}_{= X^T y}$$

$$\Rightarrow (X^T X + \lambda_C I_{D+1}) \hat{\theta}_{REG} = X^T y$$

$$\Rightarrow \hat{\theta}_{REG} = (X^T X + \lambda_C I_{D+1})^{-1} X^T y$$

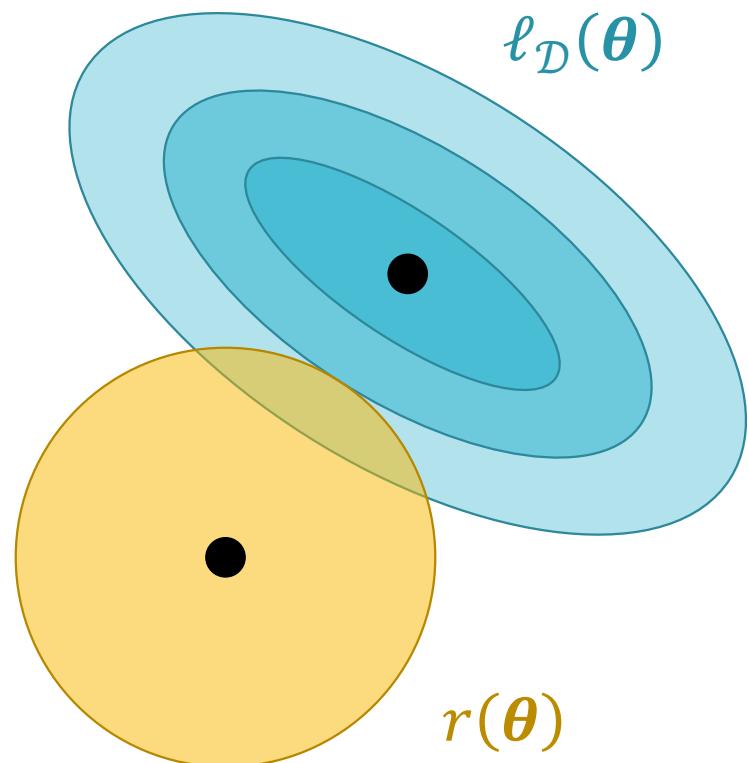
51

Poll Question 3

TOXIC

X F

- Suppose we are minimizing $\ell_D^{AUG}(\theta) = \ell_D(\theta) + \lambda_C \underline{r(\theta)}$.
As λ_C increases, the minimum of ℓ_D^{AUG} ...
- A. ... moves towards the midpoint of ℓ_D and r
- B. ... moves towards the minimum of ℓ_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

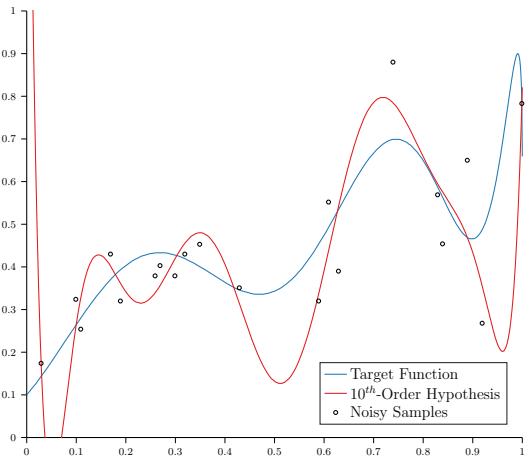


Regularization: Q & A

- Should we regularize the bias/intercept parameter, θ_0 ?
- Is feature scale a concern with regularization?

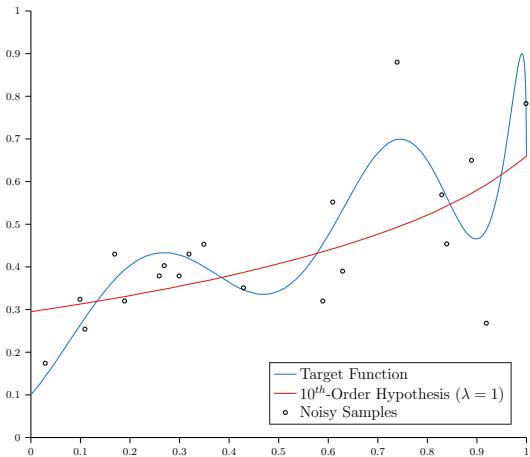
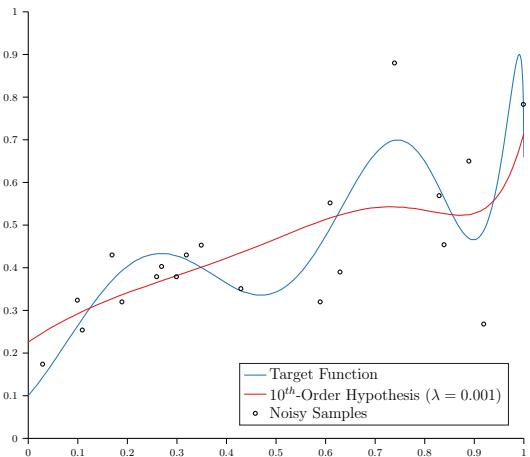
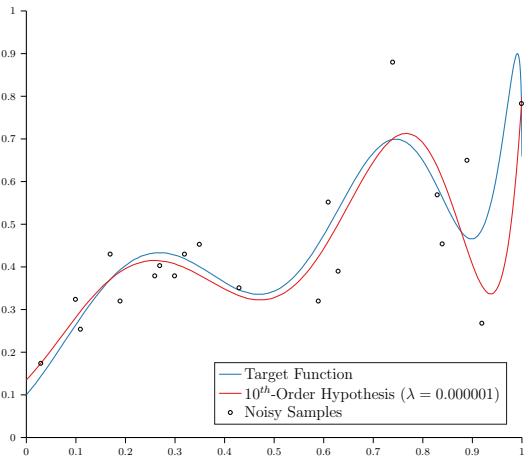
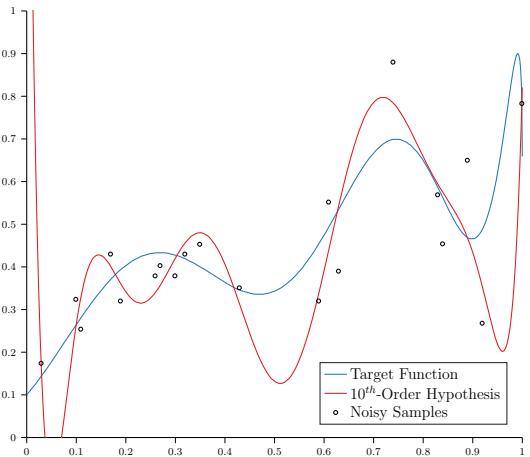
Regularization: Best Practices

- Should we regularize the bias/intercept parameter, θ_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



$$\lambda_C = 0 \quad \lambda_C = 10^{-6} \quad \lambda_C = 10^{-3} \quad \lambda_C = 1$$

Ridge Regression

True
Error

0.059	0.006	0.008	0.011
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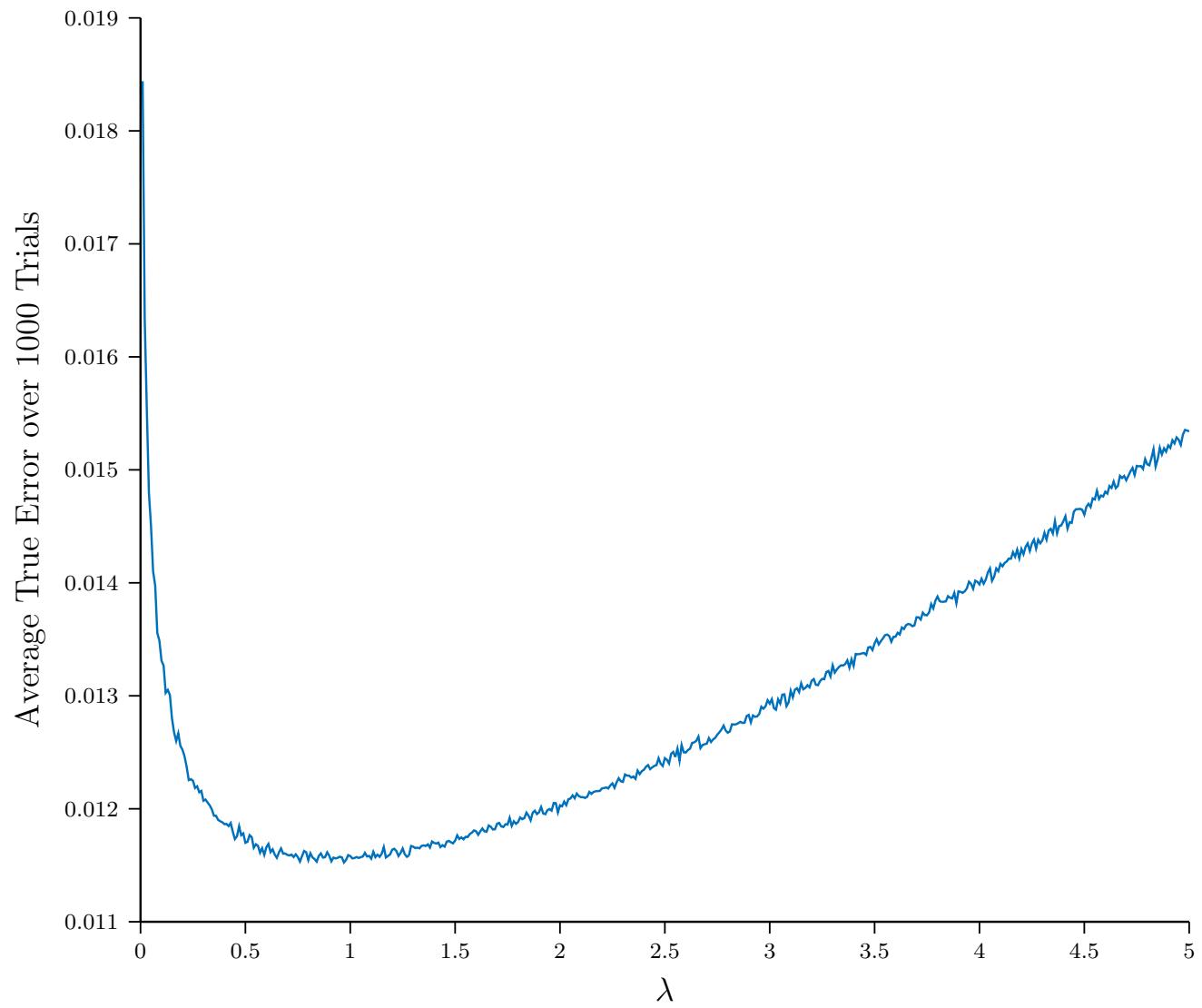
Overfit

Nice!

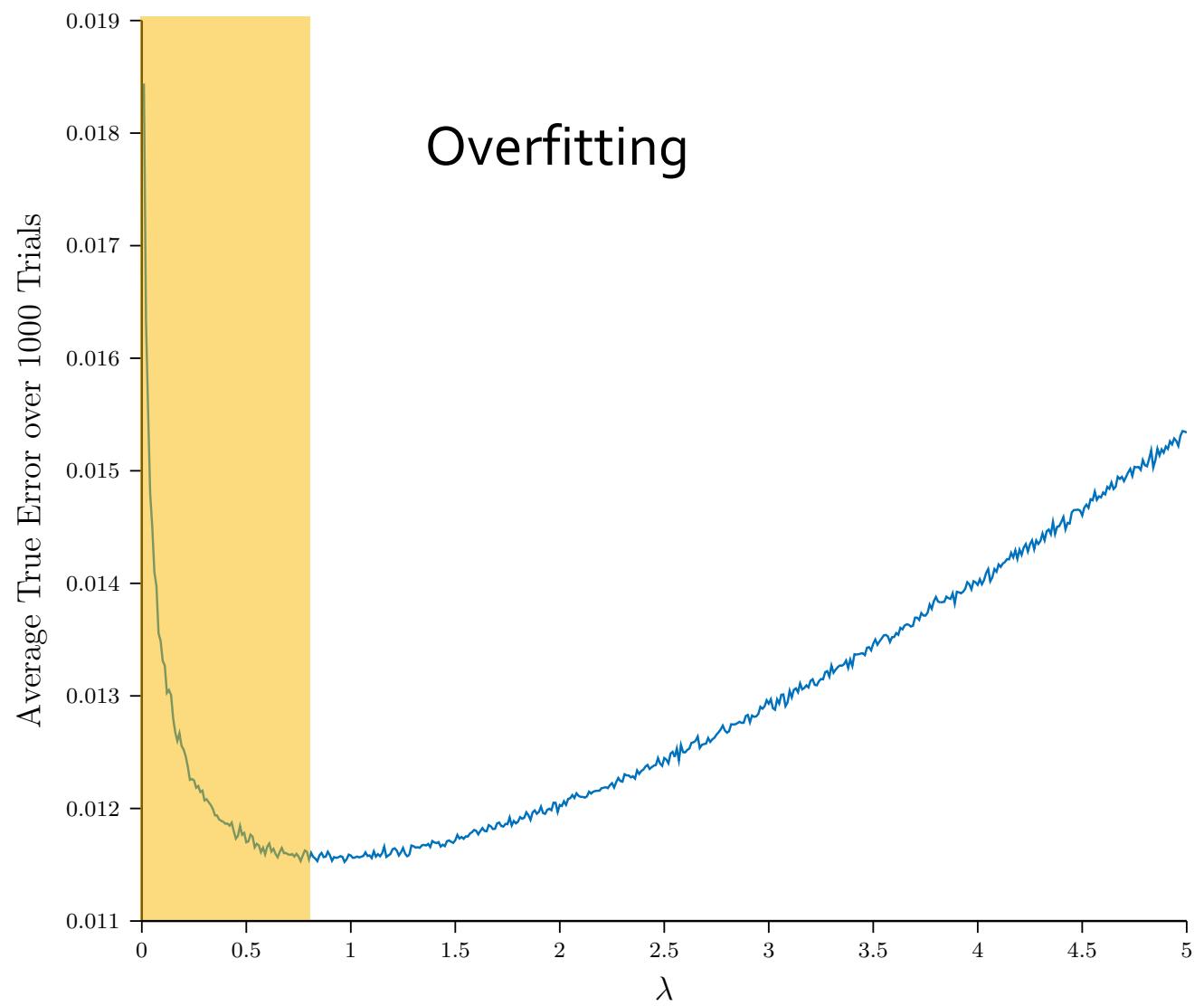
Wait...

Underfit

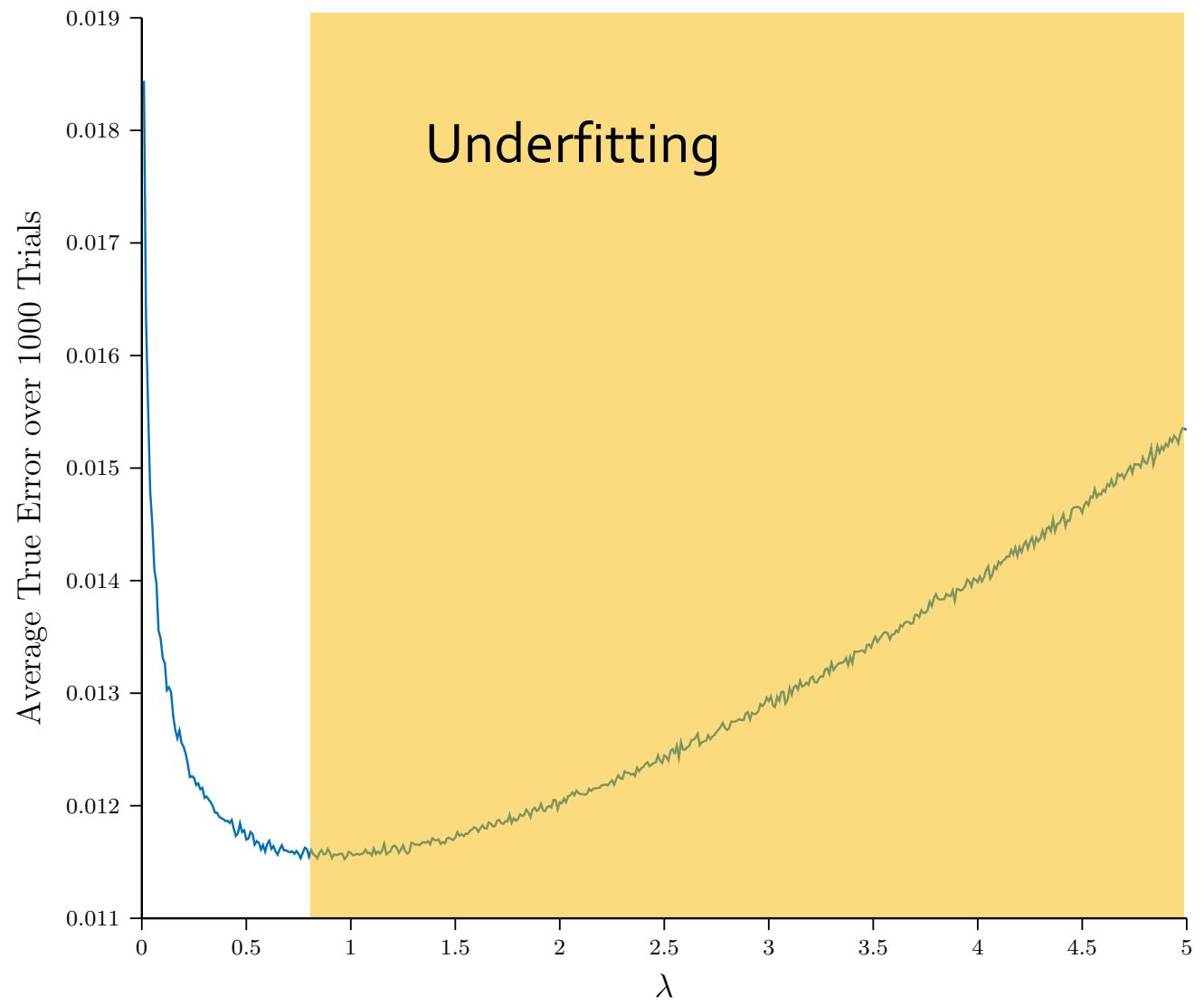
Setting λ



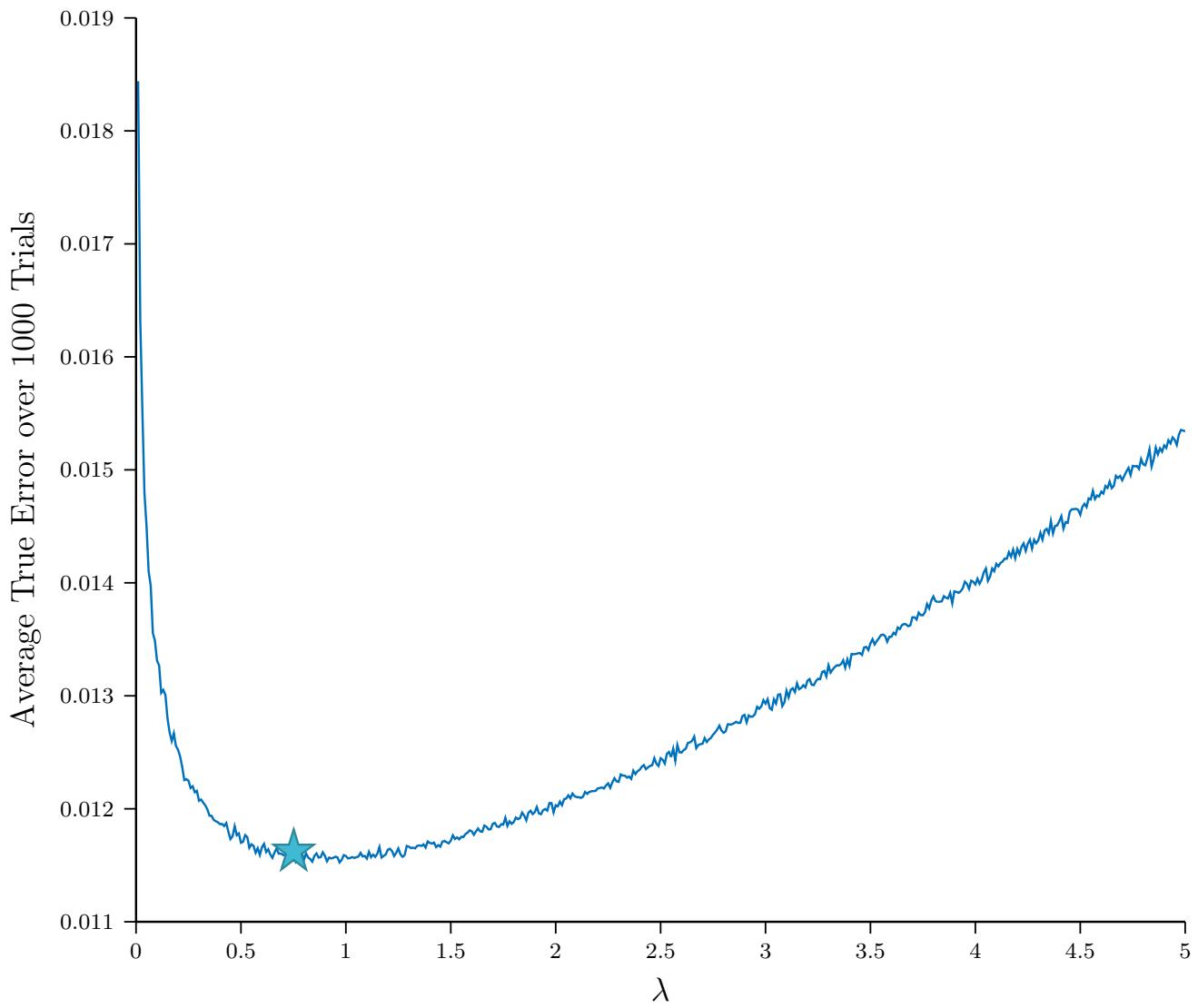
Setting λ



Setting λ



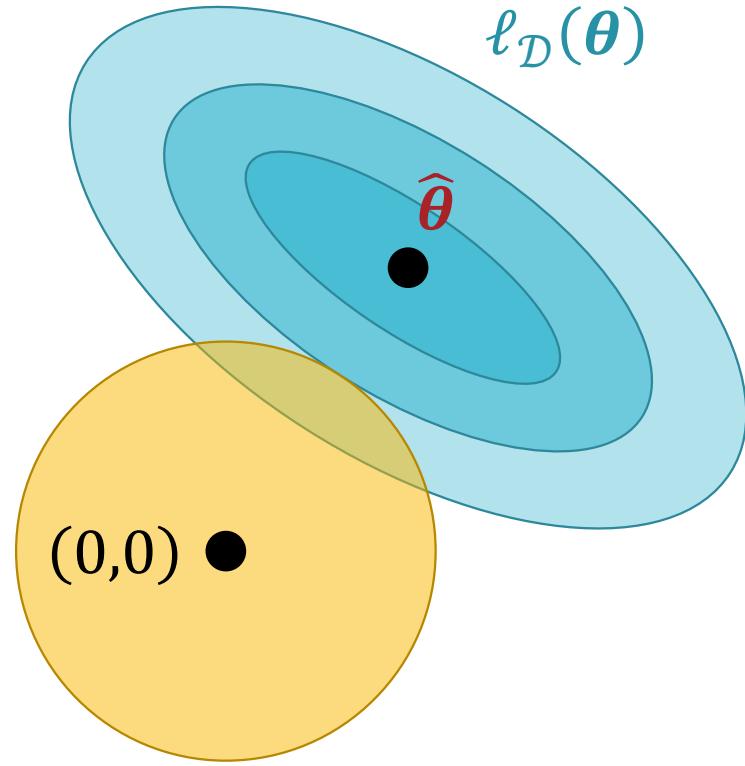
Setting λ



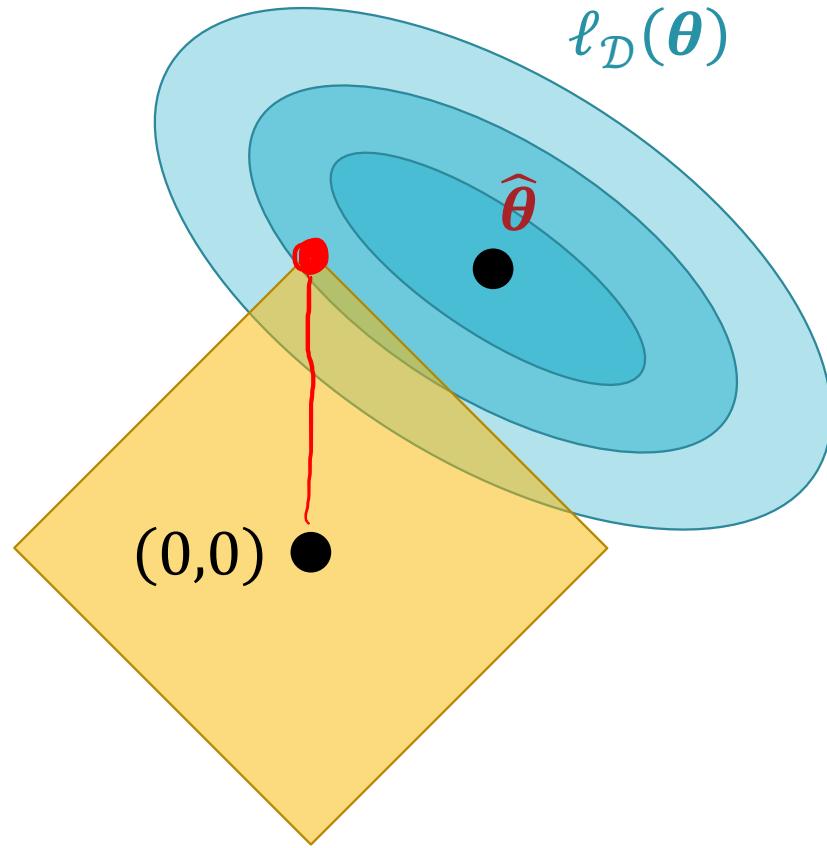
Other Regularizers

To solve in closed-form

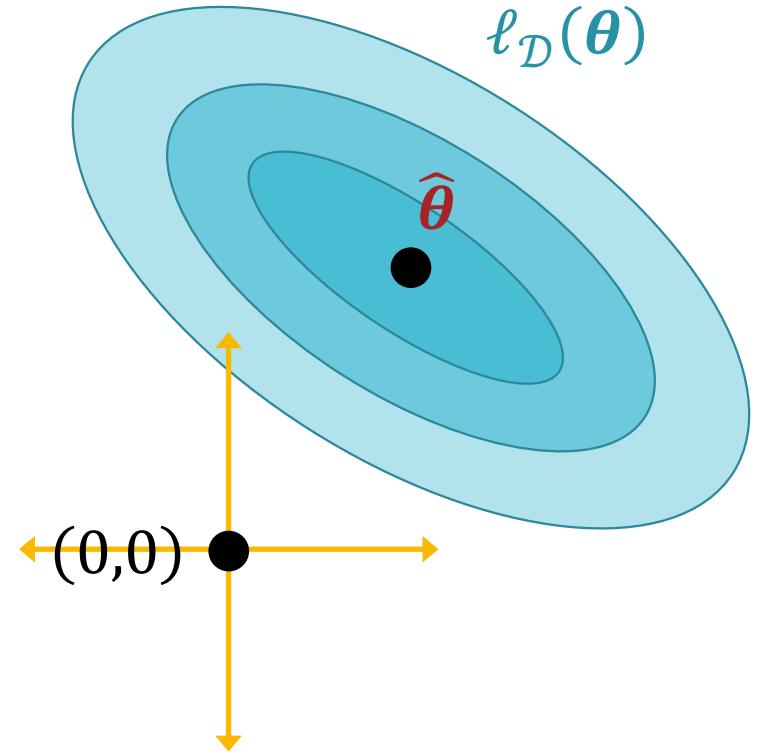
$\ell_{\mathcal{D}}(\boldsymbol{\theta}) + \lambda r(\boldsymbol{\theta})$			
Ridge or $L2$	$r(\boldsymbol{\theta}) = \ \boldsymbol{\theta}\ _2^2 = \sum_{d=0}^D \theta_d^2$		Encourages small weights
Lasso or $L1$	$r(\boldsymbol{\theta}) = \ \boldsymbol{\theta}\ _1 = \sum_{d=0}^D \theta_d $		Encourages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