10-701: Introduction to Machine Learning

Lecture 7 –Logistic Regression

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* Slides adopted from F24 offering of 10701 by Henry Chai.

Recall: Probabilistic Learning

- Previously:
  - (Unknown) Target function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$
  - Classifier, $h : \mathcal{X} \rightarrow \mathcal{Y}$
  - Goal: find a classifier, h, that best approximates c^*
- Now:
  - (Unknown) Target *distribution*, $y \sim P^*(Y|\boldsymbol{x})$
  - Distribution, $P(Y|\boldsymbol{x})$
  - Goal: find a distribution, P, that best approximates P^*

Recipe for Naïve Bayes

- Define a model space and model parameters
  - Make the Naïve Bayes assumption

$$P(X|Y) = \prod_{d=1}^{D} P(X_d|Y)$$

  - Parameters: $\pi = P(Y = 1)$, $\theta_{d,y} = P(X_d = 1|Y = y)$
- Write down an objective function
  - Maximize the log-likelihood
- Optimize the objective w.r.t. the model parameters
  - Solve in *closed form*: take partial derivatives, set to 0 and solve

Bernoulli Naïve Bayes

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {N_{Y=1}}/{N}$
    - N = # of data points
    - $N_{Y=1}$ = # of data points with label 1
- Binary features
  - $X_d | Y = y \sim \text{Bernoulli}\left(\theta_{d,y}\right)$
  - $\hat{\theta}_{d,y} = {N_{Y=y,\, X_d=1}}/{N_{Y=y}}$
    - $N_{Y=y}$ = # of data points with label y
    - $N_{Y=y,\, X_d=1}$ = # of data points with label y and feature $X_d = 1$

Bernoulli Naïve Bayes: Making Predictions

- Given a test data point $\boldsymbol{x}' = [x_1', \dots, x_D']^T$

Bernoulli Naïve Bayes: Making Predictions

- Given a test data point $\boldsymbol{x}' = [x'_1, \dots, x'_D]^T$

$$P(Y = 1|\boldsymbol{x}') \propto P(Y = 1)P(\boldsymbol{x}'|Y = 1)$$

$$= \hat{\pi} \prod_{d=1}^{D} \hat{\theta}_{d,1}^{x'_d} \left(1 - \hat{\theta}_{d,1}\right)^{1-x'_d}$$

$$P(Y = 0|\boldsymbol{x}') \propto (1 - \hat{\pi}) \prod_{d=1}^{D} \hat{\theta}_{d,0}^{x'_d} \left(1 - \hat{\theta}_{d,0}\right)^{1-x'_d}$$

$$\hat{y} = \begin{cases} 1 \text{ if } \hat{\pi} \prod_{d=1}^{D} \hat{\theta}_{d,1}^{x'_d} \left(1 - \hat{\theta}_{d,1}\right)^{1-x'_d} > \\ \quad (1 - \hat{\pi}) \prod_{d=1}^{D} \hat{\theta}_{d,0}^{x'_d} \left(1 - \hat{\theta}_{d,0}\right)^{1-x'_d} \\ 0 \text{ otherwise} \end{cases}$$

What if some Word-Label pair never appears in our training data?

x_1 ("hat")	x_2 ("cat")	x_3 ("dog")	x_4 ("fish")	x_5 ("mom")	x_6 ("dad")	y (Dr. Seuss)
1	1	0	0	0	0	1
0	0	1	0	0	0	0
0	0	0	1	0	0	1
0	0	0	0	1	0	0

The Cat in the Hat gets a Dog (by ???)

- If some $\hat{\theta}_{d,y} = 0$ and that word appears in our test data $\boldsymbol{x}'$, then $P(Y = y|\boldsymbol{x}') = 0$ even if all the other features in $\boldsymbol{x}'$ point to the label being y!
- The model has been overfit to the training data...
- We can address this with a prior over the parameters!

Setting the Parameters via MAP

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {}^{N_{Y=1}}/_{N}$
    - N = # of data points
    - $N_{Y=1}$ = # of data points with label 1
- Binary features
  - $X_d | Y = y \sim \text{Bernoulli}\left(\theta_{d,y}\right)$ and $\theta_{d,y} \sim \text{Beta}(\alpha, \beta)$
  - $\hat{\theta}_{d,y} = {}^{N_{Y=y,\, X_d=1}+(\alpha-1)}/_{N_{Y=y}+(\alpha-1)+(\beta-1)}$
    - $N_{Y=y}$ = # of data points with label y
    - $N_{Y=y,\, X_d=1}$ = # of data points with label y and feature $X_d = 1$
    - α and β are “pseudocounts” of imagined data points that help avoid zero-probability predictions.
    - Common choice: $\alpha = \beta = 2$

What can we do when this is a bad/incorrect assumption, e.g., when our features are words in a sentence?

- ***Assume*** features are conditionally independent given the label:

$$P(X|Y) = \prod_{d=1}^{D} P(X_d|Y)$$

- Pros:
  - Significantly reduces computational complexity
  - Also reduces model complexity, combats overfitting
- Cons:
  - Is a strong, often illogical assumption
    - We'll see a relaxed version of this much later when we discuss Bayesian networks

Key Takeaways

- Text data
  - Bag-of-words feature representation
- Naïve Bayes
  - Conditional independence assumption
    - Pros and cons
  - Different Naïve Bayes models based on type of features
  - MLE vs. MAP for Bernoulli Naïve Bayes

Recall: Building a Probabilistic Classifier

- Define a decision rule
  - Given a test data point $\boldsymbol{x}'$, predict its label $\hat{y}$ using the *posterior distribution* $P(Y = y|X = \boldsymbol{x}')$
  - Common choice: $\hat{y} = \underset{y}{\operatorname{argmax}}\, P(Y = y|X = \boldsymbol{x}')$
- Model the posterior distribution
  - Option 1 - Model $P(Y|X)$ directly as some function of X (today!)
  - Option 2 - Use Bayes' rule (Monday):

$$P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)} \propto P(X|Y)\,P(Y)$$

Modelling the Posterior

- Suppose we have binary labels $y \in \{0,1\}$ and D-dimensional inputs $\boldsymbol{x} = [1, x_1, \dots, x_D]^T \in \mathbb{R}^{D+1}$
- **Assume**

- This implies two useful facts:

Modelling the Posterior

- Suppose we have binary labels $y \in \{0,1\}$ and D-dimensional inputs $\boldsymbol{x} = [1, x_1, \dots, x_D]^T \in \mathbb{R}^{D+1}$
- **Assume**

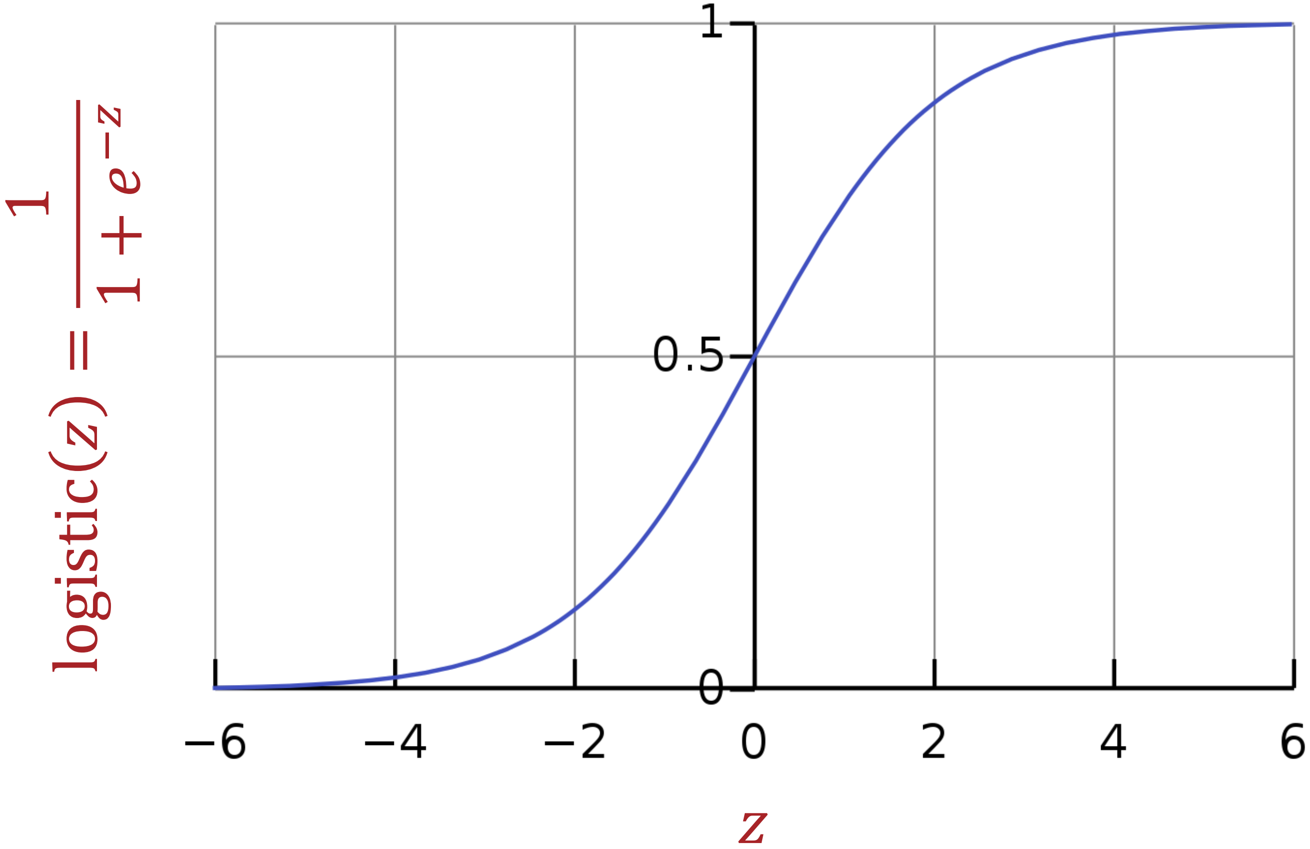
$$P(Y = 1|\boldsymbol{x}) = \text{logistic}(\boldsymbol{w}^T\boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T\boldsymbol{x})}$$

$$= \frac{\exp(\boldsymbol{w}^T\boldsymbol{x})}{\exp(\boldsymbol{w}^T\boldsymbol{x}) + 1}$$

- This implies two useful facts:

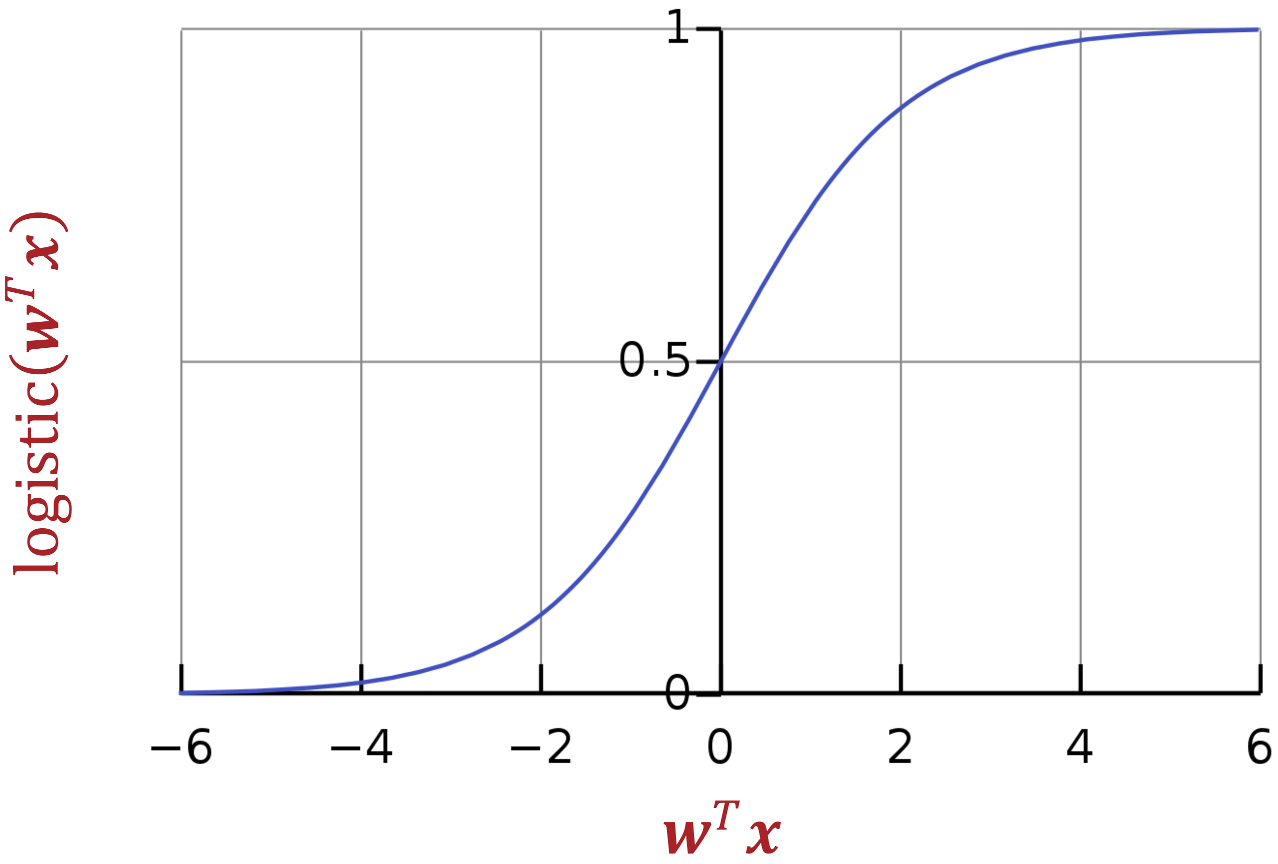
1. $P(Y = 0|\boldsymbol{x}) = 1 - P(Y = 1|\boldsymbol{x}) = \dfrac{1}{\exp(\boldsymbol{w}^T\boldsymbol{x}) + 1}$
2. $\dfrac{P(Y = 1|\boldsymbol{x})}{P(Y = 0|\boldsymbol{x})} = \exp(\boldsymbol{w}^T\boldsymbol{x}) \rightarrow \log\dfrac{P(Y = 1|\boldsymbol{x})}{P(Y = 0|\boldsymbol{x})} = \boldsymbol{w}^T\boldsymbol{x}$

Logistic Function



Source: https://en.wikipedia.org/wiki/Logistic_function#/media/File:Logistic-curve.svg

Why use the Logistic Function?



- Differentiable everywhere
- logistic: $\mathbb{R} \rightarrow [0, 1]$

Source: https://en.wikipedia.org/wiki/Logistic_function#/media/File:Logistic-curve.svg

Logistic Regression Decision Boundary

The decision boundary is linear in $\boldsymbol{x}$!

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$$\hat{y} = \begin{cases} 1 \text{ if } P(Y = 1|\boldsymbol{x}) \geq \frac{1}{2} \\ 0 \text{ otherwise} \end{cases}$$

$$P(Y = 1|\boldsymbol{x}) = \text{logistic}(\boldsymbol{w}^T\boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T\boldsymbol{x})} \geq \frac{1}{2}$$

$$2 \geq 1 + \exp(-\boldsymbol{w}^T\boldsymbol{x})$$

$$1 \geq \exp(-\boldsymbol{w}^T\boldsymbol{x})$$

$$\log(1) \geq -\boldsymbol{w}^T\boldsymbol{x}$$

$$0 \leq \boldsymbol{w}^T\boldsymbol{x}$$

Logistic Regression Decision Boundary

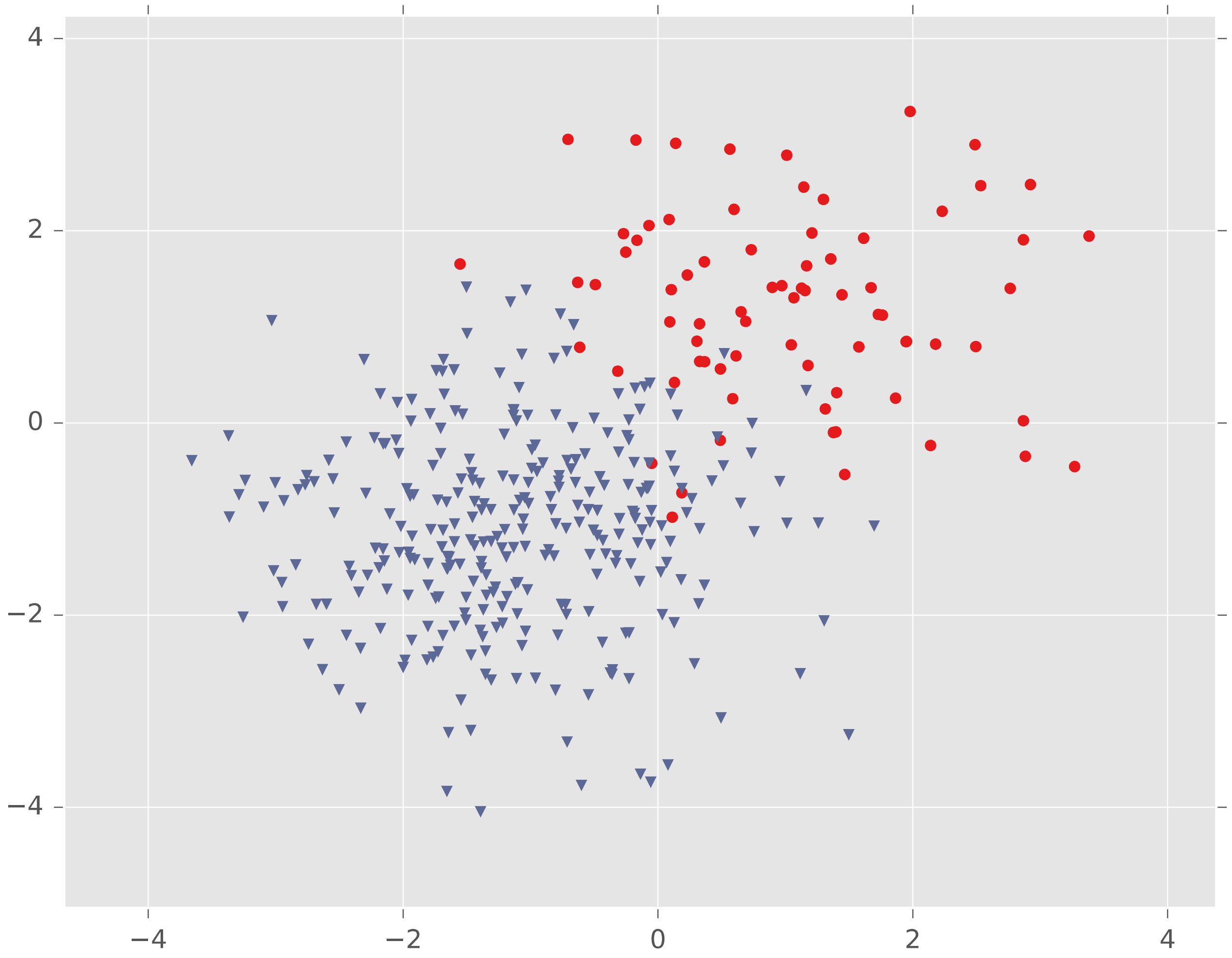

Figure courtesy of Matt Gormley

Logistic Regression Decision Boundary

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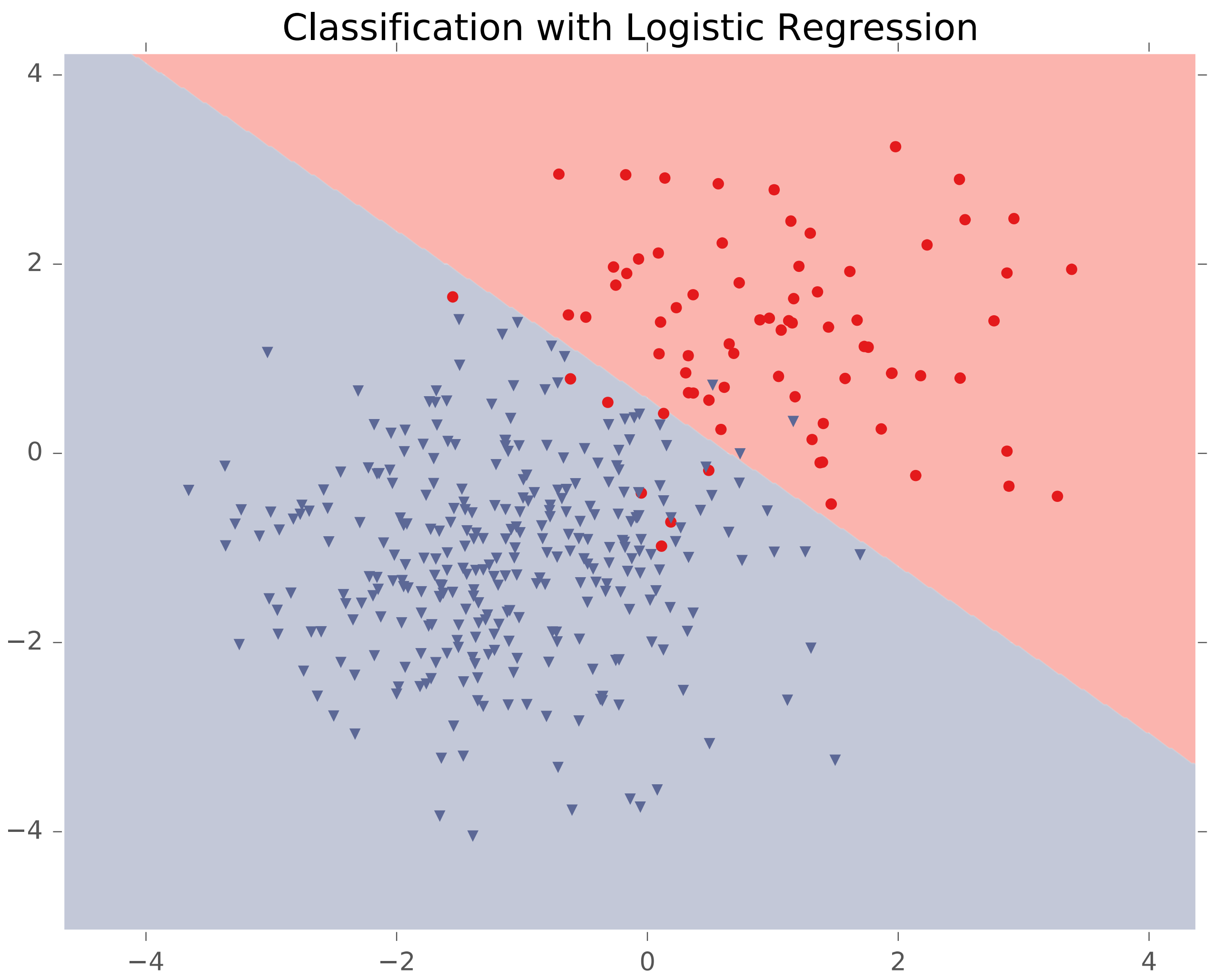


Figure courtesy of Matt Gormley

General Recipe for Machine Learning

- Define a model space and model parameters

- Write down an objective function

- Optimize the objective w.r.t. the model parameters

Recipe for Logistic Regression

- Define a model space and model parameters
  - Assume independent, identically distributed (iid) data
  - Assume $P(Y = 1|X) = \text{logistic}(\boldsymbol{w}^T\boldsymbol{x})$
  - Parameters: $\boldsymbol{w} = [w_0, w_1, \dots, w_D]$
- Write down an objective function
  - ~~Maximize the *conditional* log-likelihood~~
  - Minimize the negative conditional log-likelihood
- Optimize the objective w.r.t. the model parameters
  - ???

Setting the Parameters via Minimum Negative Conditional (log-)Likelihood Estimation (MCLE)

Find $\boldsymbol{w}$ that minimizes

$$\ell_{\mathcal{D}}(\boldsymbol{w}) =$$

Setting the Parameters via Minimum Negative Conditional (log-)Likelihood Estimation (MCLE)

Find $\boldsymbol{w}$ that minimizes

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = -\log P\left(y^{(1)}, \dots, y^{(N)} \middle| \boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}, \boldsymbol{w}\right) = -\log \prod_{n=1}^{N} P\left(y^{(n)} \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)$$

$$= -\log \prod_{n=1}^{N} P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)^{y^{(n)}} \left(P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)\right)^{1-y^{(n)}}$$

$$= -\sum_{n=1}^{N} y^{(n)} \log P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right) + \left(1 - y^{(n)}\right) \log P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)$$

$$= -\sum_{n=1}^{N} y^{(n)} \log \frac{P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)}{P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)} + \log P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right)$$

$$= -\sum_{n=1}^{N} y^{(n)} \boldsymbol{w}^T \boldsymbol{x}^{(n)} - \log\left(1 + \exp\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)\right)$$

Minimizing the Negative Conditional (log-)Likelihood

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = -\sum_{n=1}^{N} y^{(n)} \boldsymbol{w}^T \boldsymbol{x}^{(n)} - \log\left(1 + \exp\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)\right)$$

Minimizing the Negative Conditional (log-)Likelihood

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = -\sum_{n=1}^{N} y^{(n)} \boldsymbol{w}^T \boldsymbol{x}^{(n)} - \log\left(1 + \exp\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)\right)$$

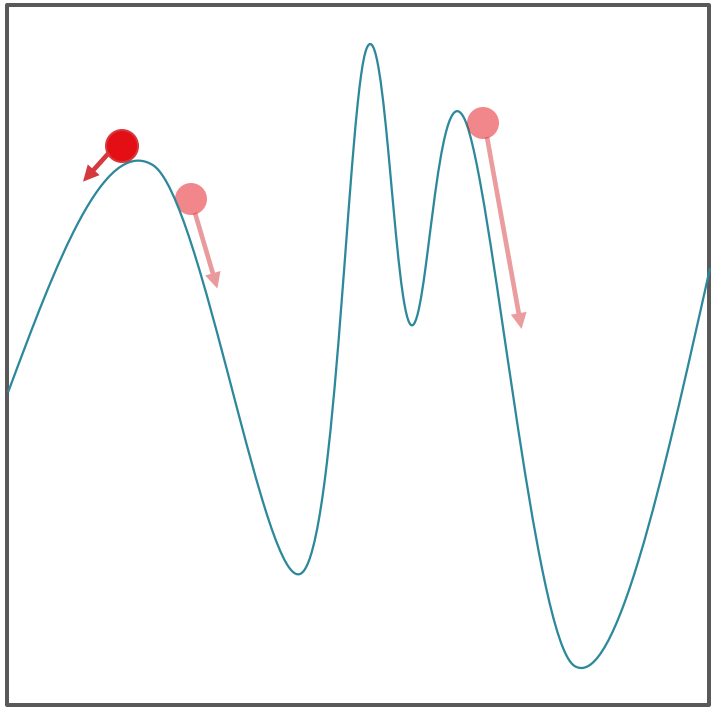
$$\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}(\boldsymbol{w}) = -\sum_{n=1}^{N} y^{(n)} \nabla_{\boldsymbol{w}} \boldsymbol{w}^T \boldsymbol{x}^{(n)} - \nabla_{\boldsymbol{w}} \log\left(1 + \exp\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)\right)$$

$$= -\sum_{n=1}^{N} y^{(n)} \boldsymbol{x}^{(n)} - \frac{\exp\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)}{1 + \exp\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)} \boldsymbol{x}^{(n)}$$

$$= \sum_{n=1}^{N} \boldsymbol{x}^{(n)} \left(P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}\right) - y^{(n)}\right)$$

Recall: Gradient Descent

- An iterative method for minimizing functions
- Requires the gradient to exist everywhere



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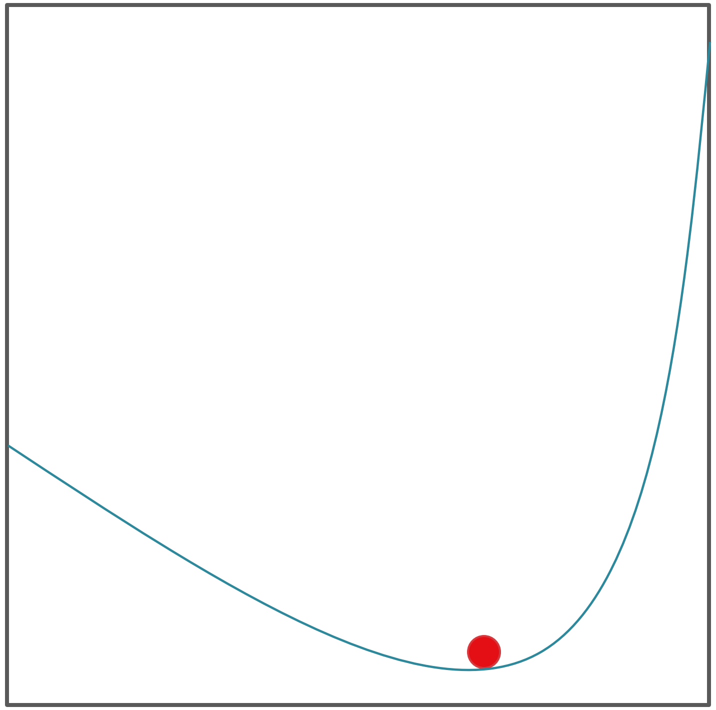


- Good news: the negative conditional log-likelihood, like the squared error, is also convex!

Gradient Descent

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}, \eta^{(0)}$

1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. Compute the gradient:

$$O(ND)\left\{\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right) = \sum_{n=1}^{N} \boldsymbol{x}^{(n)}\left(P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}^{(t)}\right) - y^{(n)}\right)\right.$$

   b. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta^{(0)} \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   c. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

Stochastic Gradient Descent

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}, \eta_{SGD}^{(0)}$

1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. Randomly sample a data point from $\mathcal{D}$, $\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)$
   b. Compute the pointwise gradient:
      $$\nabla_{\boldsymbol{w}}\ell^{(n)}\left(\boldsymbol{w}^{(t)}\right) = \boldsymbol{x}^{(n)}\left(P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}^{(t)}\right) - y^{(n)}\right)$$
   c. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta_{SGD}^{(0)}\nabla_{\boldsymbol{w}}\ell^{(n)}\left(\boldsymbol{w}^{(t)}\right)$
   d. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

Stochastic Gradient Descent

- If the data point is sampled uniformly at random, then the expected value of the pointwise gradient is proportional to the full gradient:

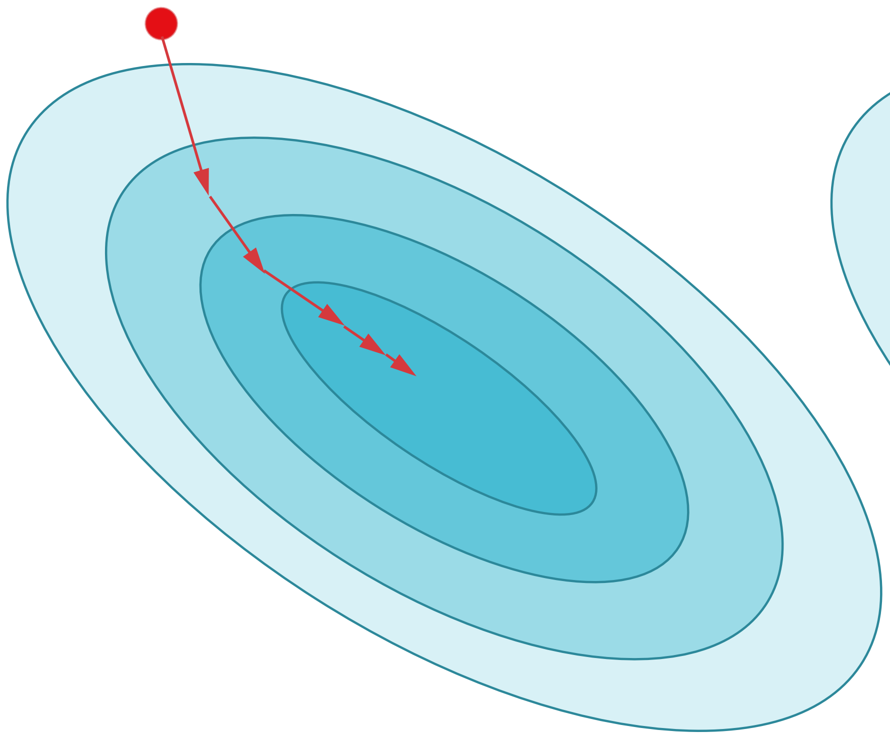
$$E\left[\nabla_{\boldsymbol{w}} \ell_{\boldsymbol{x}^{(n)}, y^{(n)}}\left(\boldsymbol{w}^{(t)}\right)\right] = \frac{1}{N} \sum_{n=1}^{N} \nabla_{\boldsymbol{w}} \ell^{(n)}\left(\boldsymbol{w}^{(t)}\right)$$

$$= \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{x}^{(n)}\left(P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{w}^{(t)}\right) - y^{(n)}\right)$$

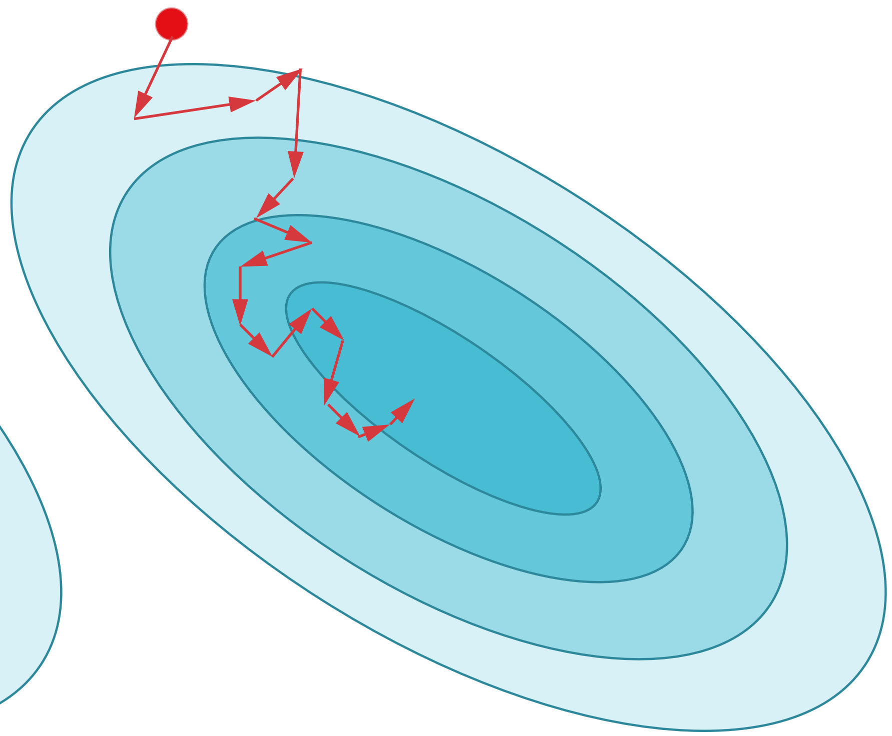
$$= \frac{1}{N} \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$$

- In practice, the data set is randomly shuffled then looped through so that each data point is used equally often

Stochastic Gradient Descent vs. Gradient Descent



Gradient Descent



Stochastic Gradient Descent

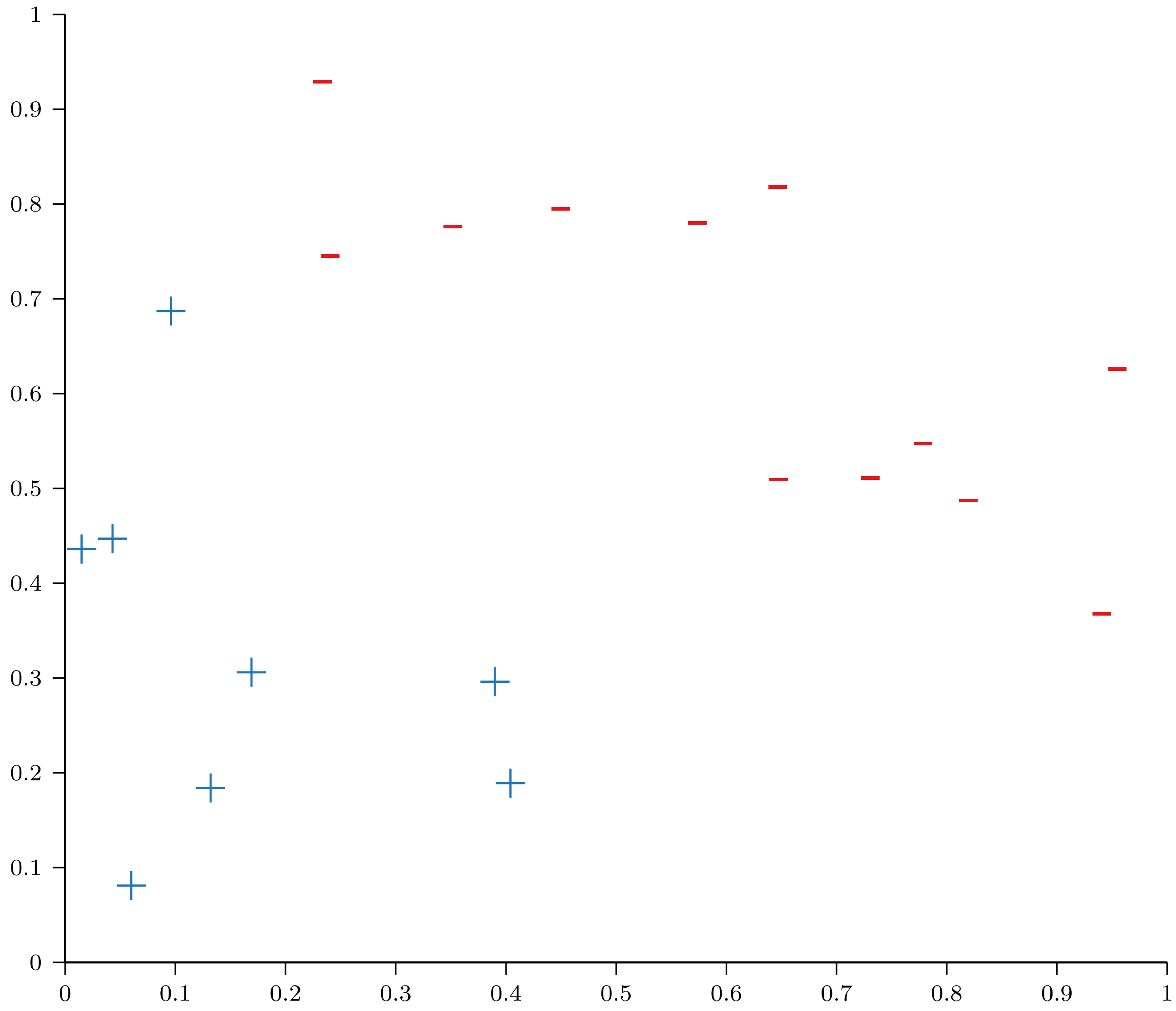
Mini-batch Stochastic Gradient Descent

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}, \eta_{MB}^{(0)}, B$

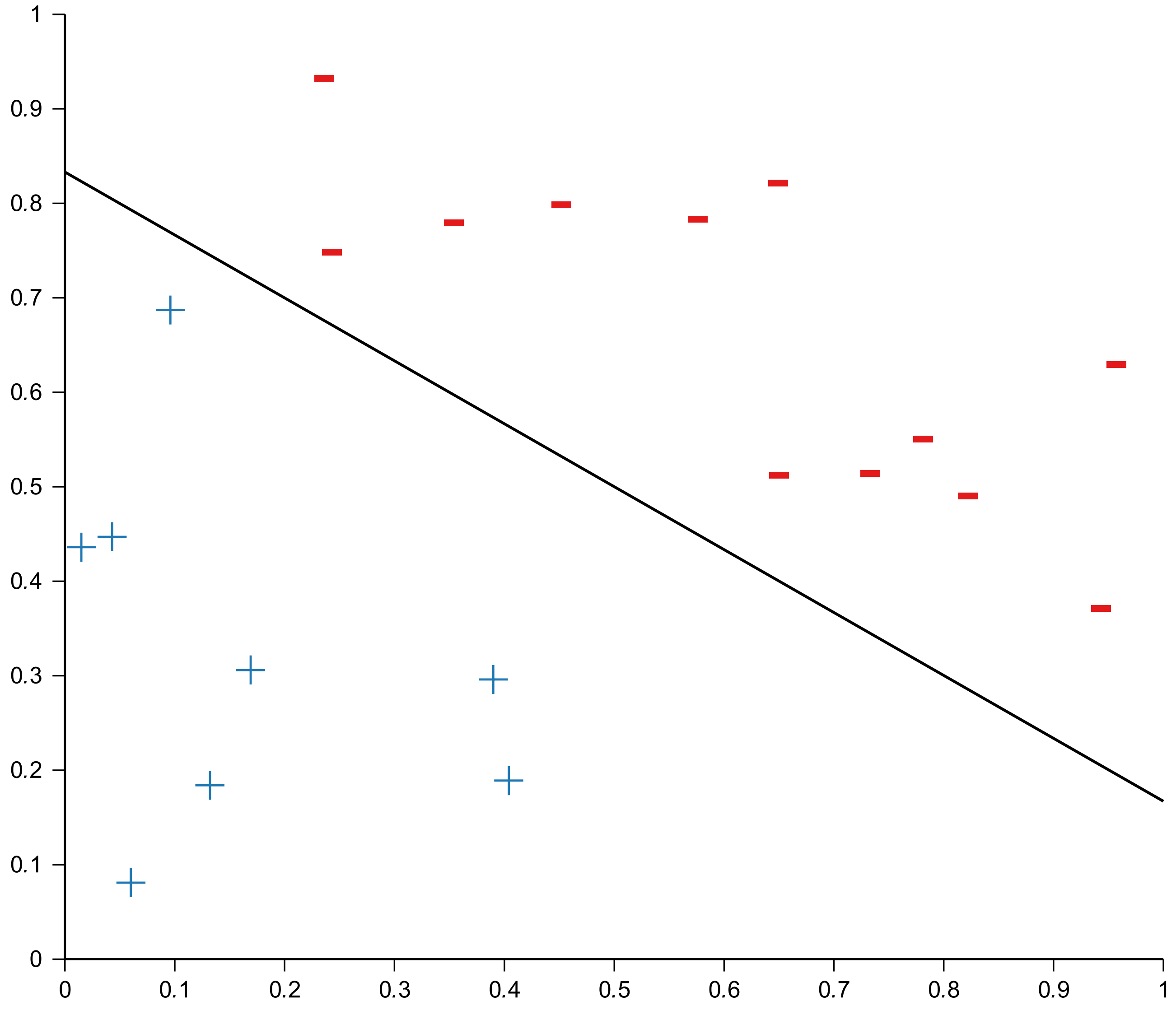
1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. Randomly sample B data points from $\mathcal{D}$:
   $$\mathcal{D}_{batch}\left\{\left(\boldsymbol{x}^{(b)}, y^{(b)}\right)\right\}_{b=1}^{B}$$
   b. Compute the gradient w.r.t. the sampled *batch*:
   $$\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}_{batch}}\left(\boldsymbol{w}^{(t)}\right) = \sum_{b=1}^{B} \boldsymbol{x}^{(b)}\left(P\left(Y = 1 \middle| \boldsymbol{x}^{(b)}, \boldsymbol{w}\right) - y^{(b)}\right)$$
   c. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta_{MB}^{(0)} \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}_{batch}}\left(\boldsymbol{w}^{(t)}\right)$
   d. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

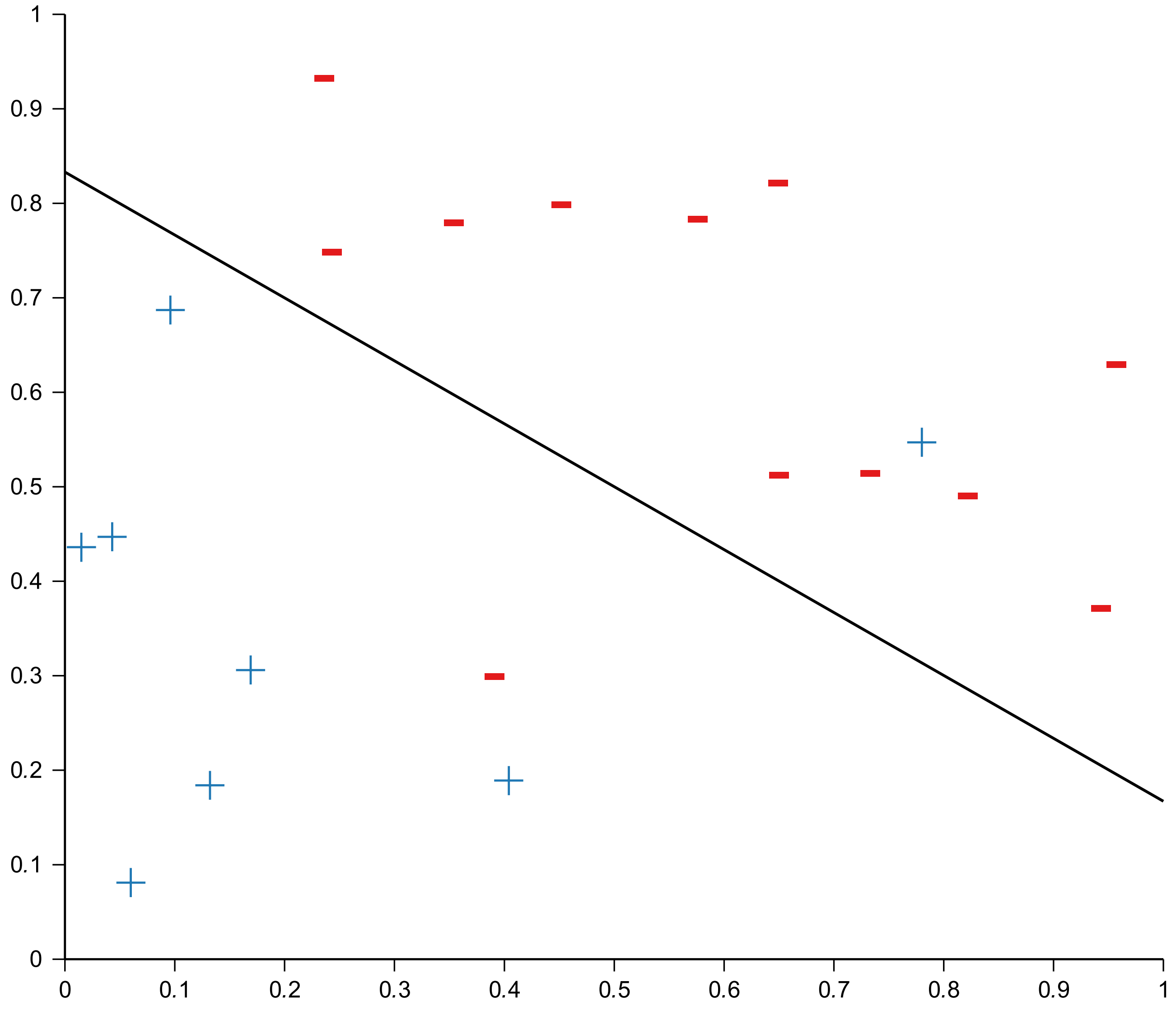
Linear Models



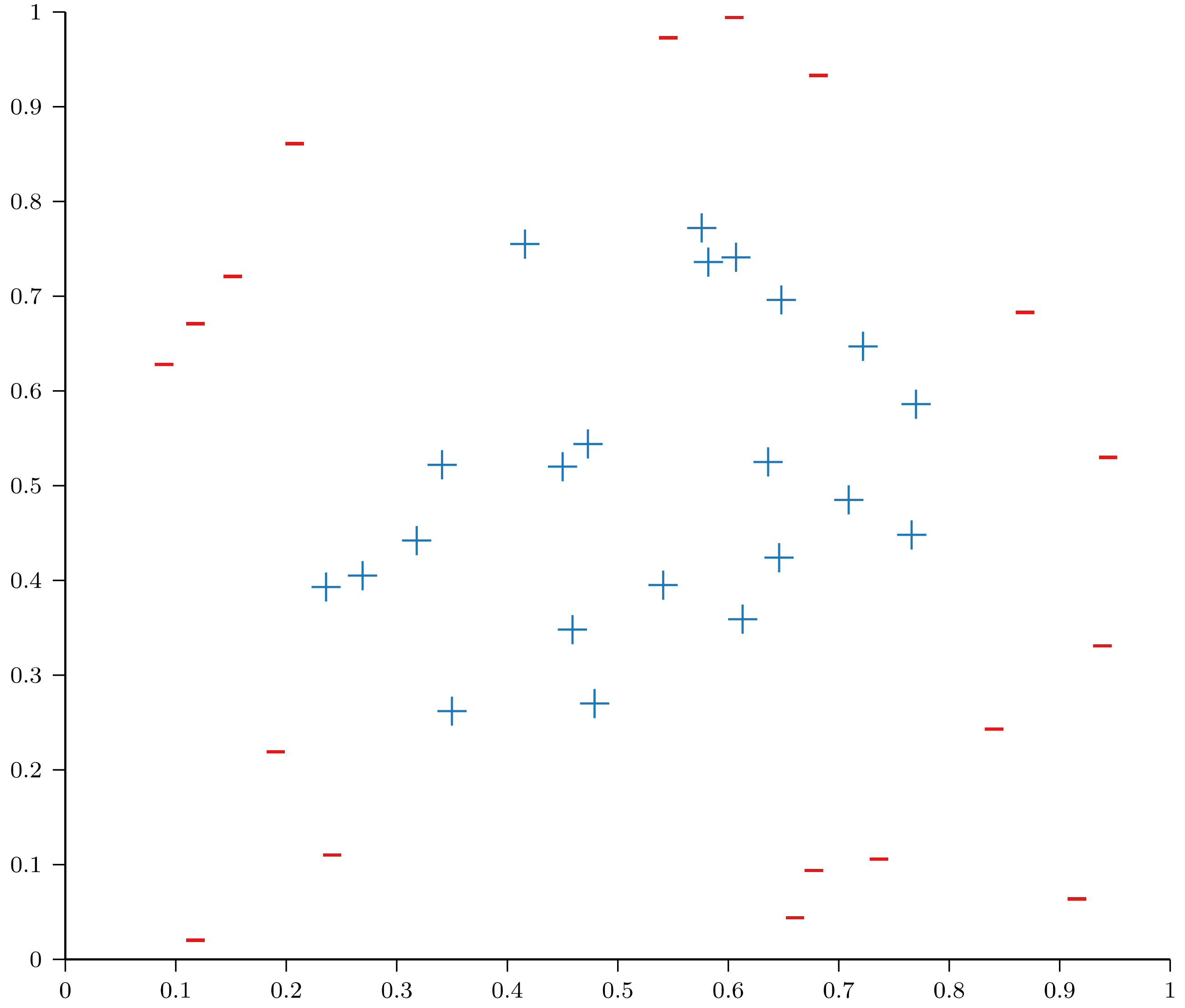
Linear Models



Linear Models



Linear Models?



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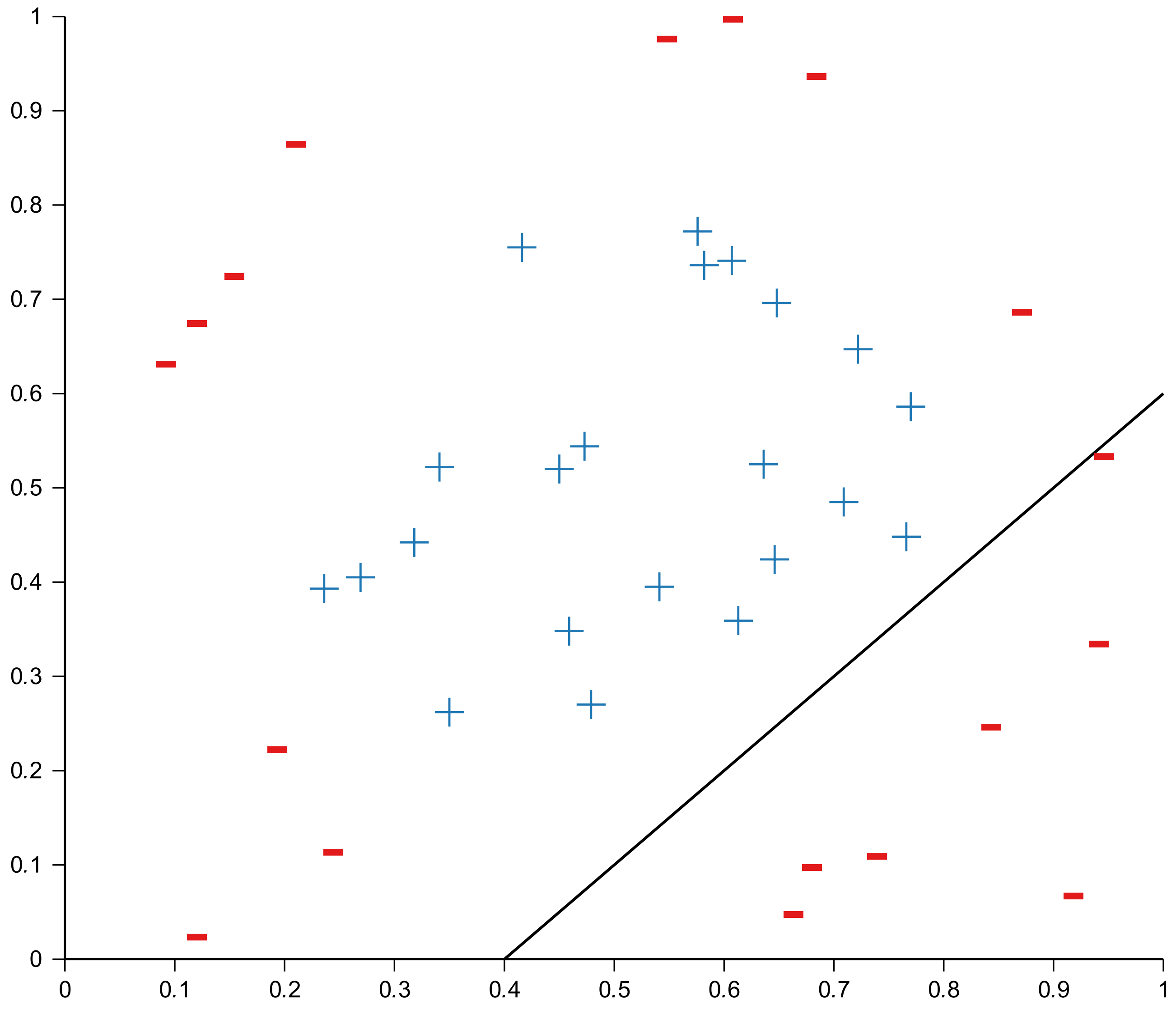
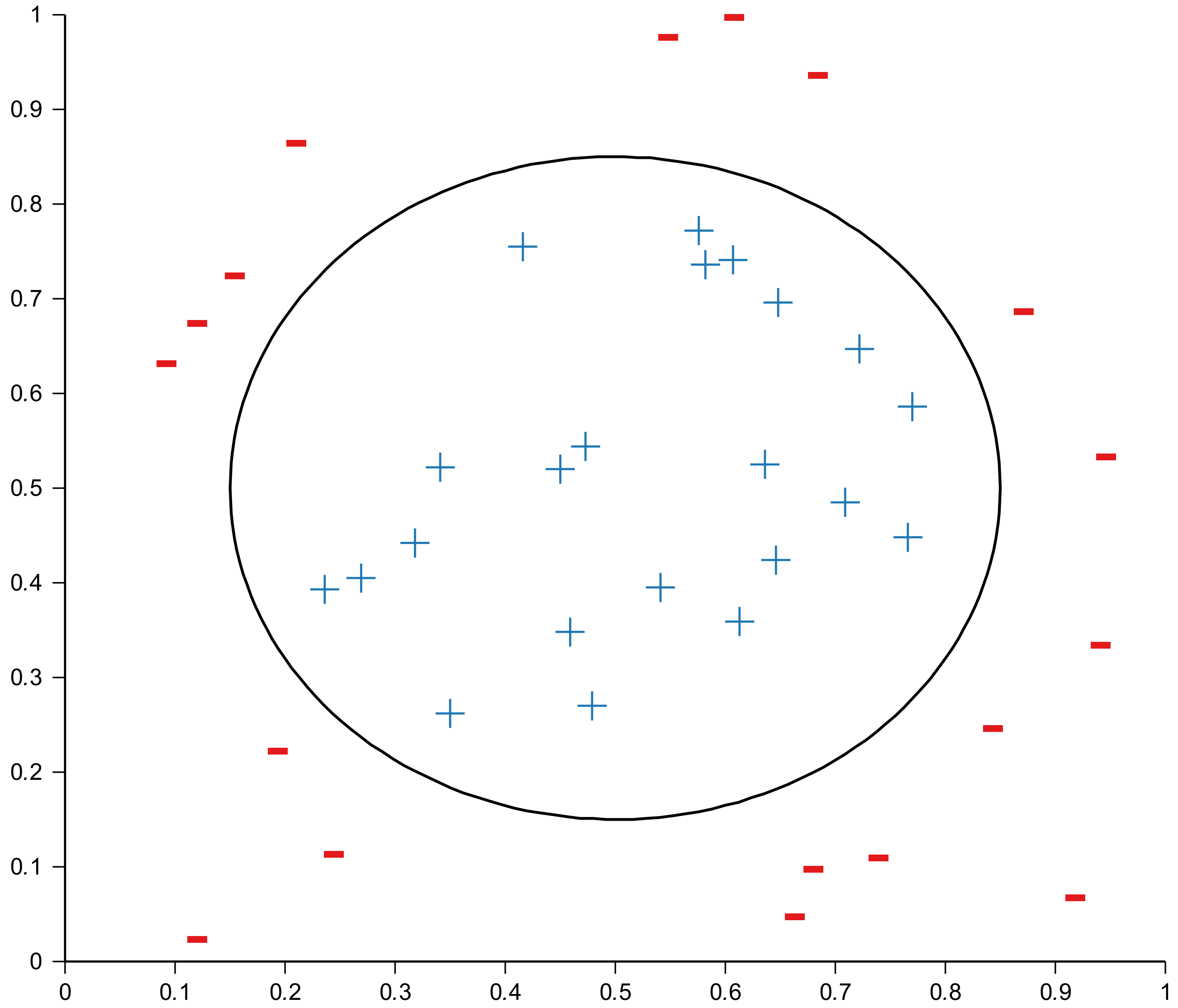


Nonlinear Models

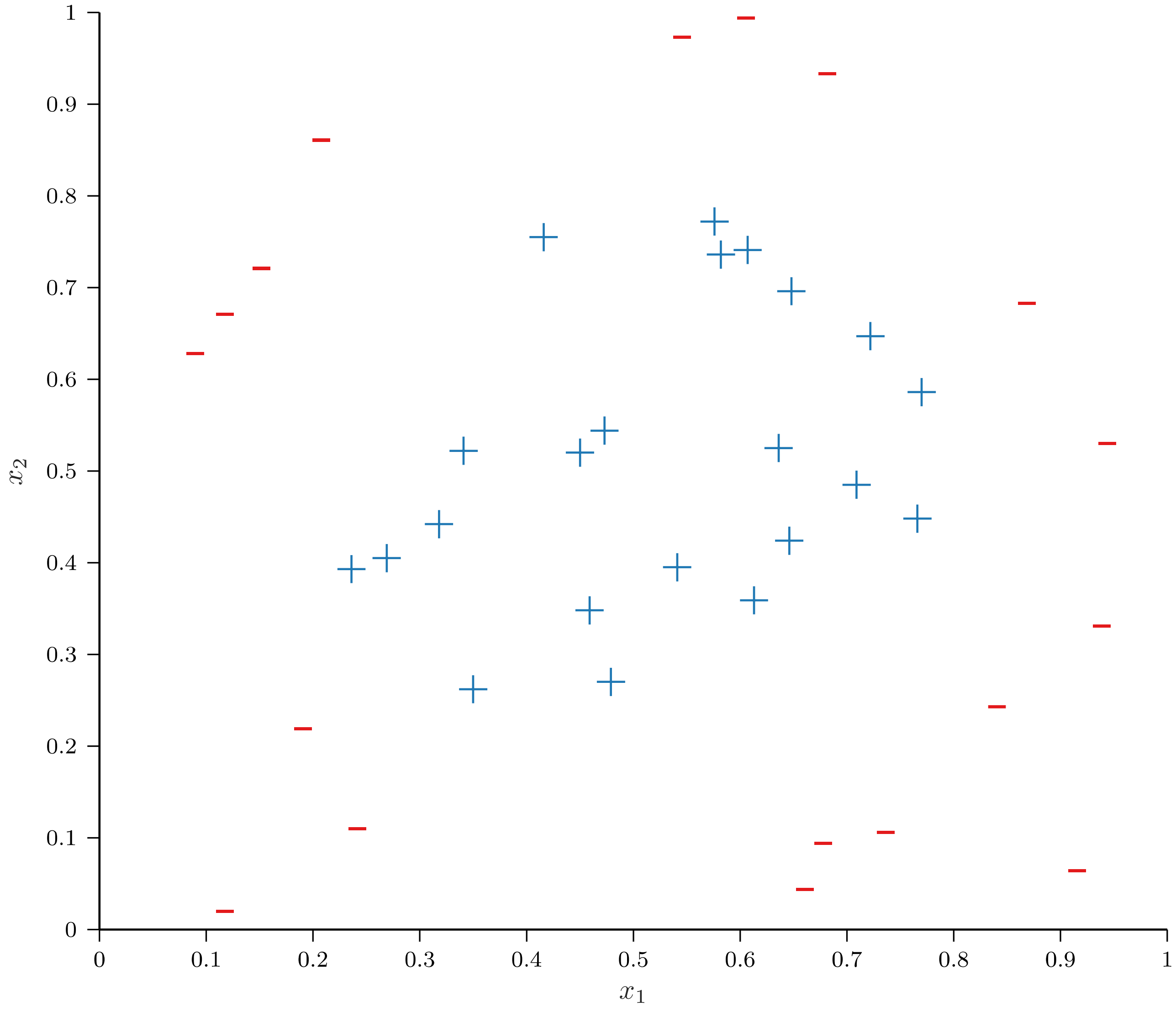


Feature Transforms

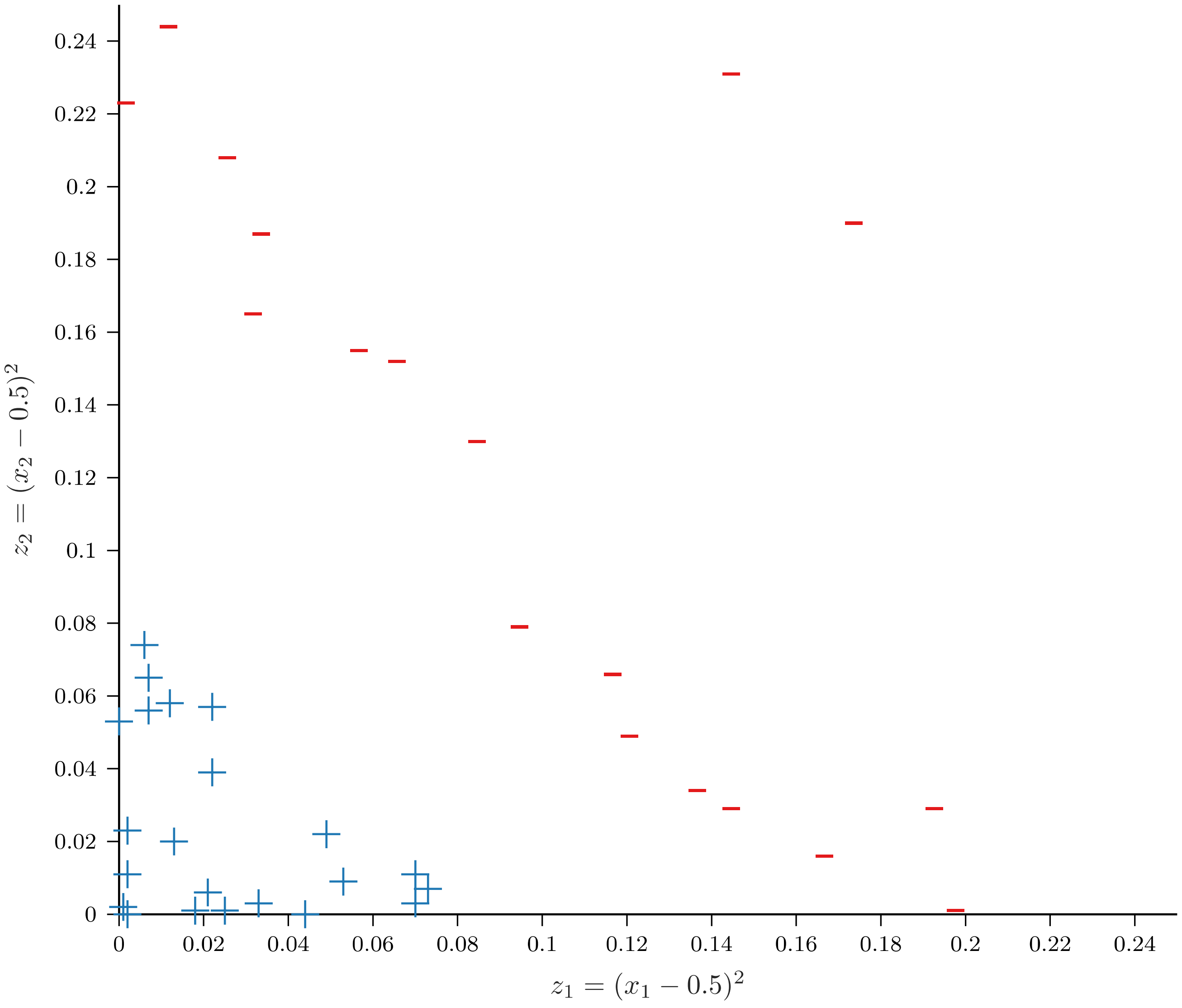
- Given D-dimensional inputs $\boldsymbol{x} = [x_1, \dots, x_D]$, first compute some transformation of our input, e.g.,

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

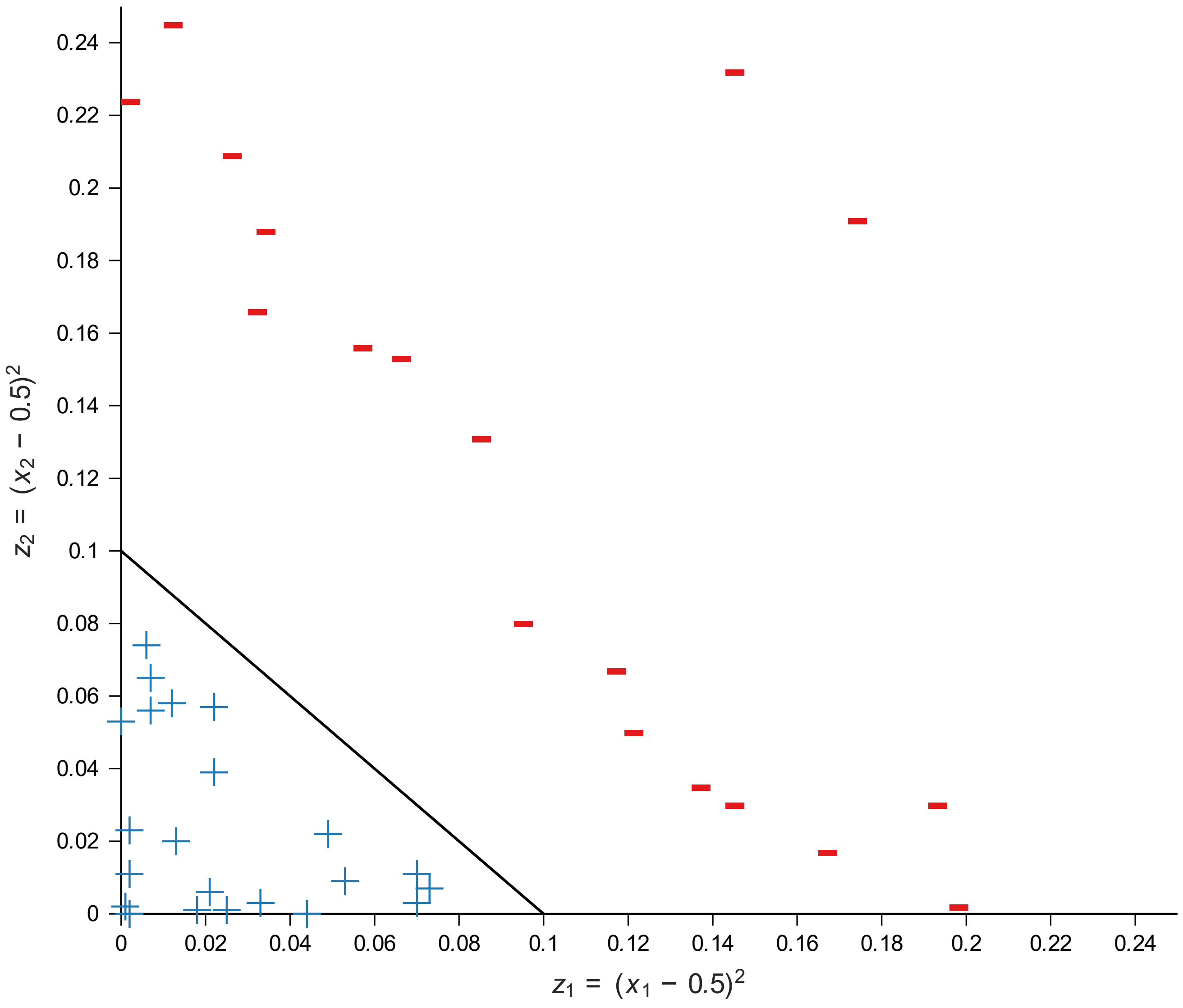
Nonlinear Models



Nonlinear Models



Nonlinear Models



Nonlinear Models