01.112/50.007 Machine Learning

Lecture 4

Regression

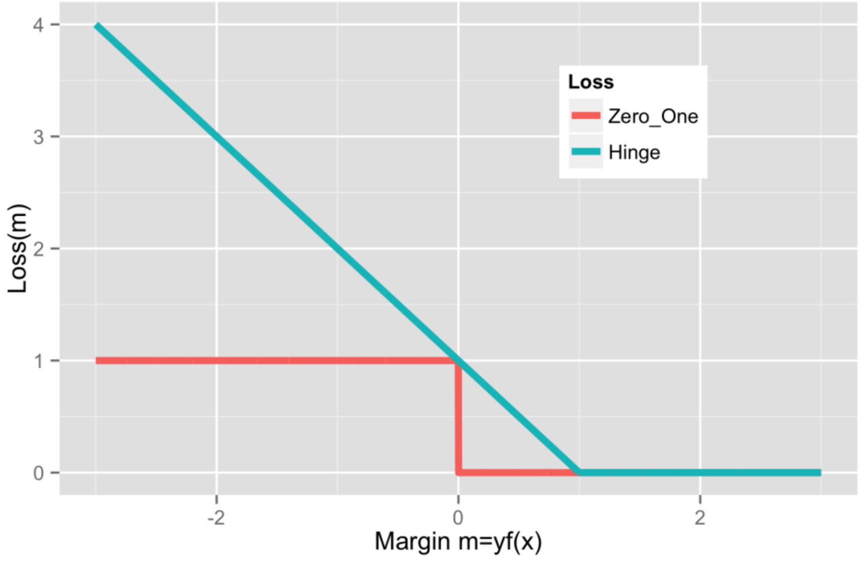
Recap

Loss Functions

- **Training Loss / Empirical risk:**

$$R_n(\theta) = \frac{1}{n} \sum_{\text{data } (x,y)} \text{Loss}\big(y(\theta^\top x)\big)$$

- **Zero-one loss:** $\text{Loss}_{0|1}(z) = [\![z \leq 0]\!]$



- **Hinge loss:** $\text{Loss}_{\text{h}}(z) = \max\{1 - z, 0\}$

CONVEX!
Penalize larger mistakes more.
Penalize near-mistakes, i.e. $0 \leq z \leq 1$.

Stochastic Gradient Descent

1. Initialize the **weight** ($\theta^{(0)} = 0$).

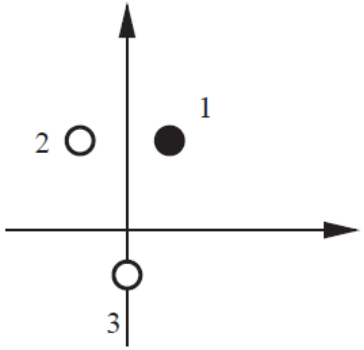
2. Select $t \in \{1, \dots, n\}$ at $\boxed{\text{random}}$

- If $\boxed{y^{(t)}(\theta^{(k)} \cdot x^{(t)}) \leq 1}$, then update the weight

$$\boxed{\theta^{(k+1)} = \theta^{(k)} + \eta_k y^{(t)} x^{(t)}}$$

3. Repeat Step (2) until stopping criterion is met.
(e.g. when improvement in $R_n(\theta)$ is small enough)

Example (Linearly Separable)



$$x^{(1)} = \begin{bmatrix}1\\2\end{bmatrix}, y^{(1)} = 1$$

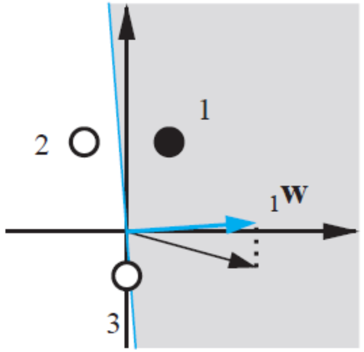
$$x^{(2)} = \begin{bmatrix}-1\\2\end{bmatrix}, y^{(2)} = -1$$

$$x^{(3)} = \begin{bmatrix}0\\-1\end{bmatrix}, y^{(3)} = -1$$

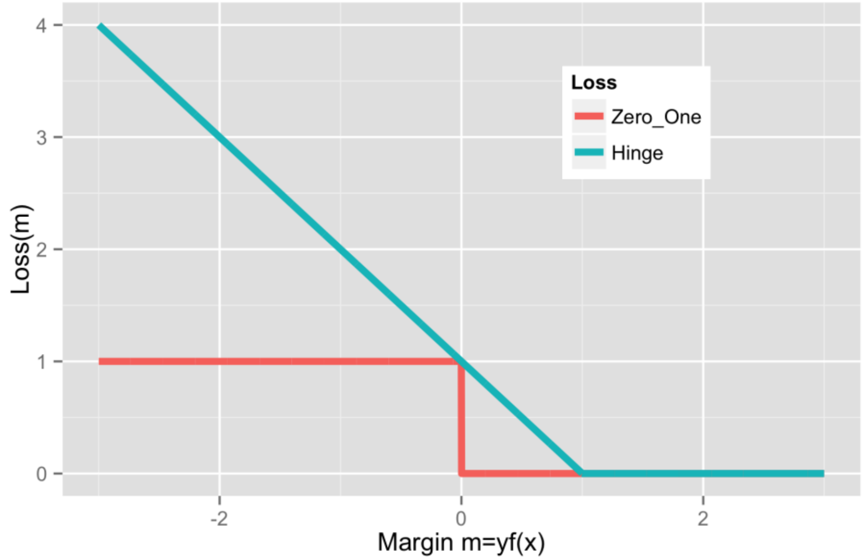
Hinge Loss:

$$R_n(\theta) = \frac{1}{n} \sum_{\text{data }(x,y)} \text{Loss}\big(y(\theta^\top x)\big)$$

$$\text{Loss}_\text{h}(z) = \max\{1 - z, 0\}$$



$$\theta^{(3)} = \begin{bmatrix}3\\0.2\end{bmatrix}$$



Linear Regression

Machine Learning

Task

Performance

Experience

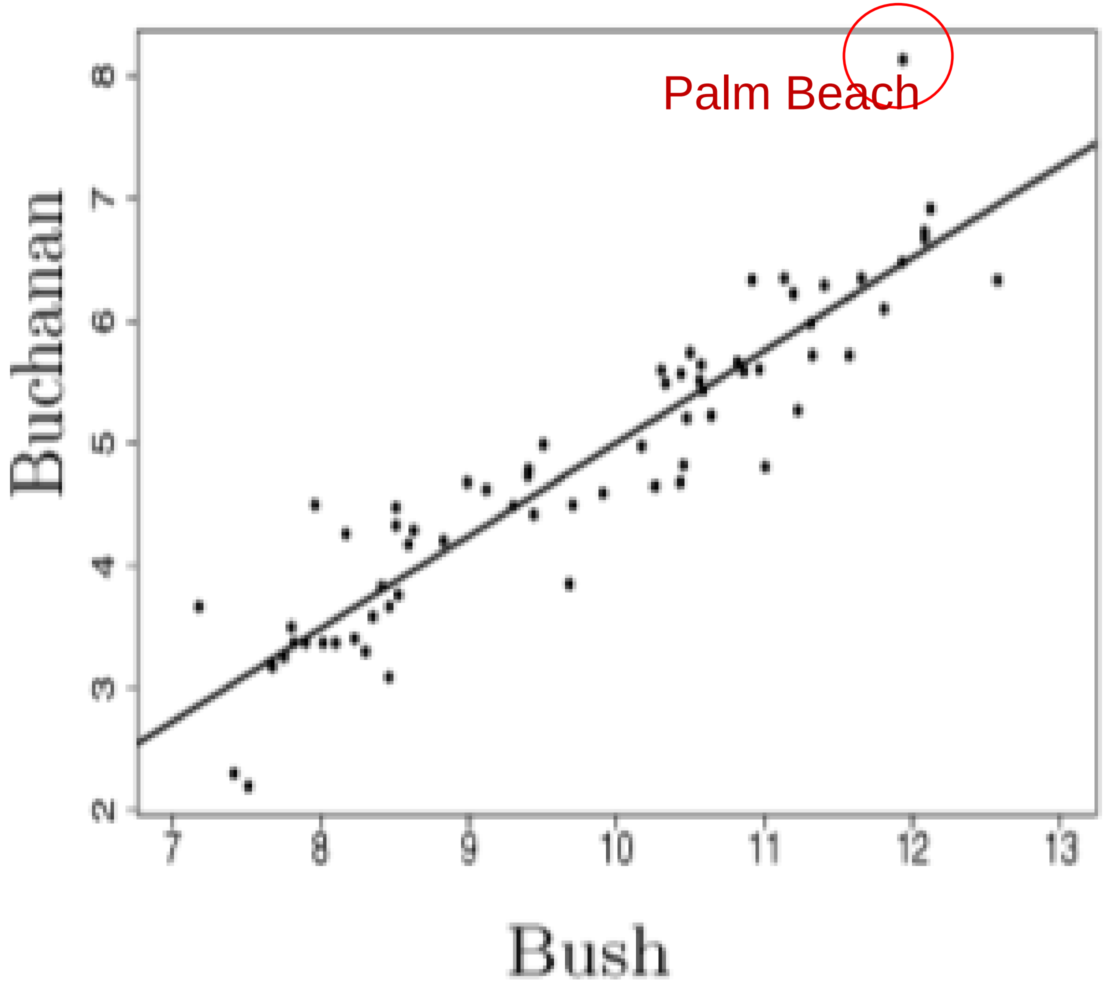
Algorithms that improve their performance at some task with experience
– Tom Mitchell (1998)

Linear Regression

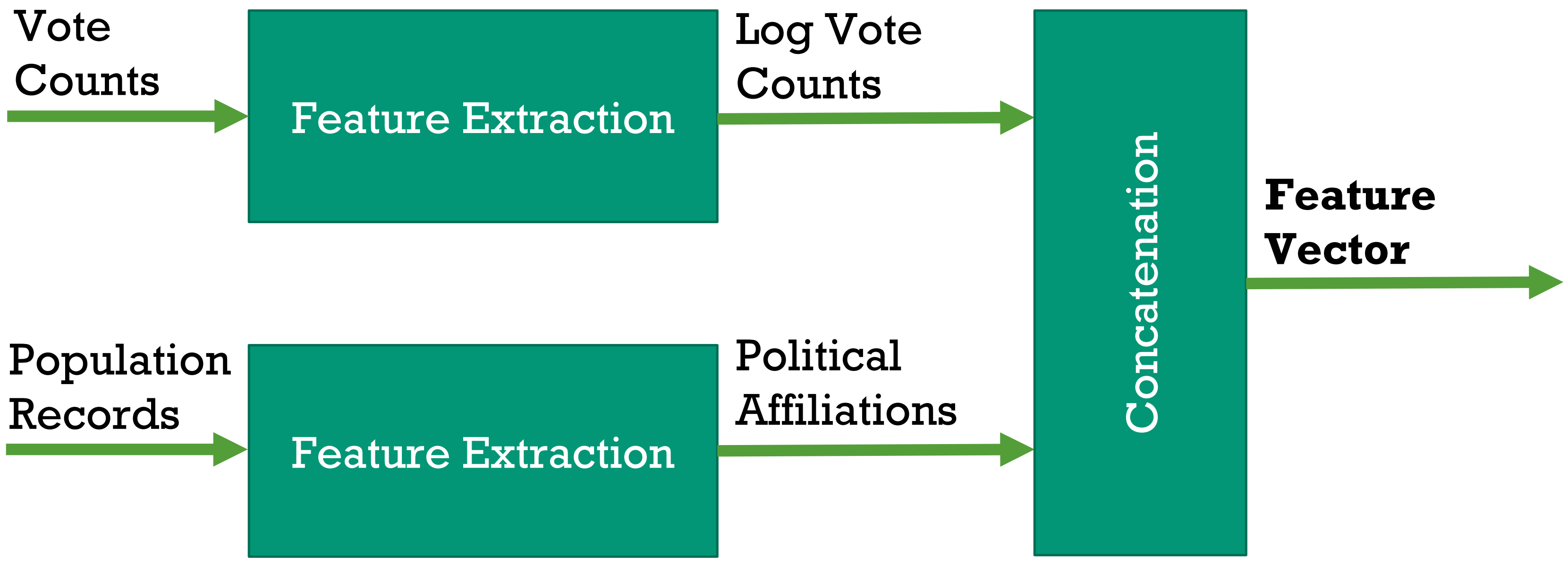
Machine Learning
> Supervised Learning
> Classification
> Regression

- **Task.** Find function $f: \mathbb{R}^d \to \mathbb{R}$ such that $y \approx f(x; \theta)$
- **Experience.** Training data $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(n)}, y^{(n)}\right)$
- **Performance.** Prediction error $y - f(x; \theta)$ on test data

Example

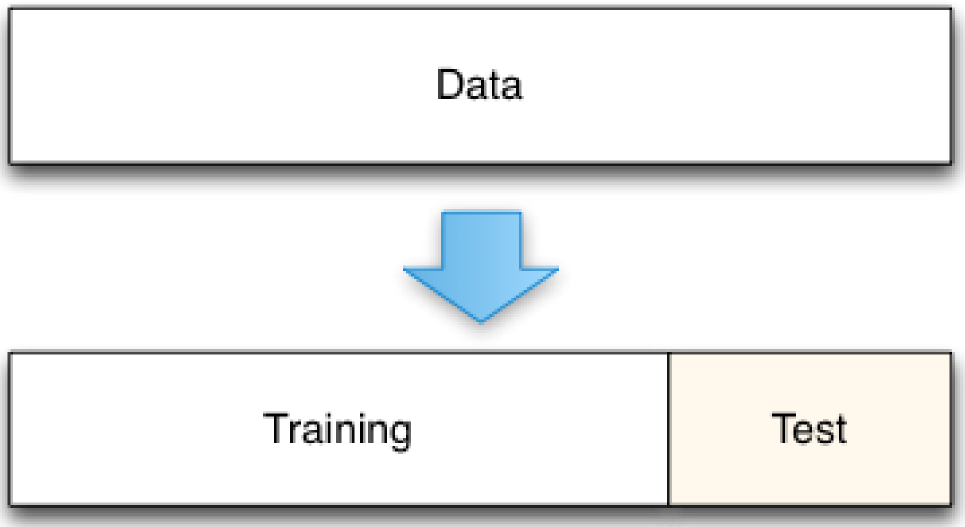


Features


Vote
Counts
Feature Extraction
Log Vote
Counts
Population
Records
Feature Extraction
Political
Affiliations
Concatenation
Feature
Vector

Training Data VS Test Data

- Partition data into:
  - Training data set $\mathcal{S}_n$
  - Test data set $\mathcal{S}_{n'}$



Linear Regression

Training data

$$\mathcal{S}_n = \left\{ \left(x^{(t)}, y^{(t)}\right) \,\middle|\, t = 1, \ldots, n \right\}$$

- Features/Inputs $x^{(t)} = \left(x_1^{(t)}, \ldots, x_d^{(t)}\right)^\top \in \mathbb{R}^d$
- Response/Output $y^{(t)} \in \mathbb{R}$

Linear Regression

Model (or Hypothesis Class) F

Each f is a *predictor* or *hypothesis*

Set of *linear* functions $f\colon \mathbb{R}^d \rightarrow \mathbb{R}$

$$f(x;\theta,\theta_0) = \theta . x = \theta_d x_d + \cdots + \theta_1 x_1 + \theta_0 = \theta^\top x + \theta_0$$

Model Parameters

$$\theta \in \mathbb{R}^d, \theta_0 \in \mathbb{R}$$

Linear Regression

- **Empirical Risk and Least Squares Criterion**

Training Loss/Objective

$$R_n(\theta) = \frac{1}{n}\sum_{t=1}^{n} \mathrm{Loss}(y^{(t)} - \theta \cdot x^{(t)}) = \frac{1}{n}\sum_{t=1}^{n} (y^{(t)} - \theta \cdot x^{(t)})^2/2$$

Training Algorithm

Find predictor $\hat{f} \in F$ that minimizes $R_n(\theta)$

The test loss and training loss can be different.

Linear Regression

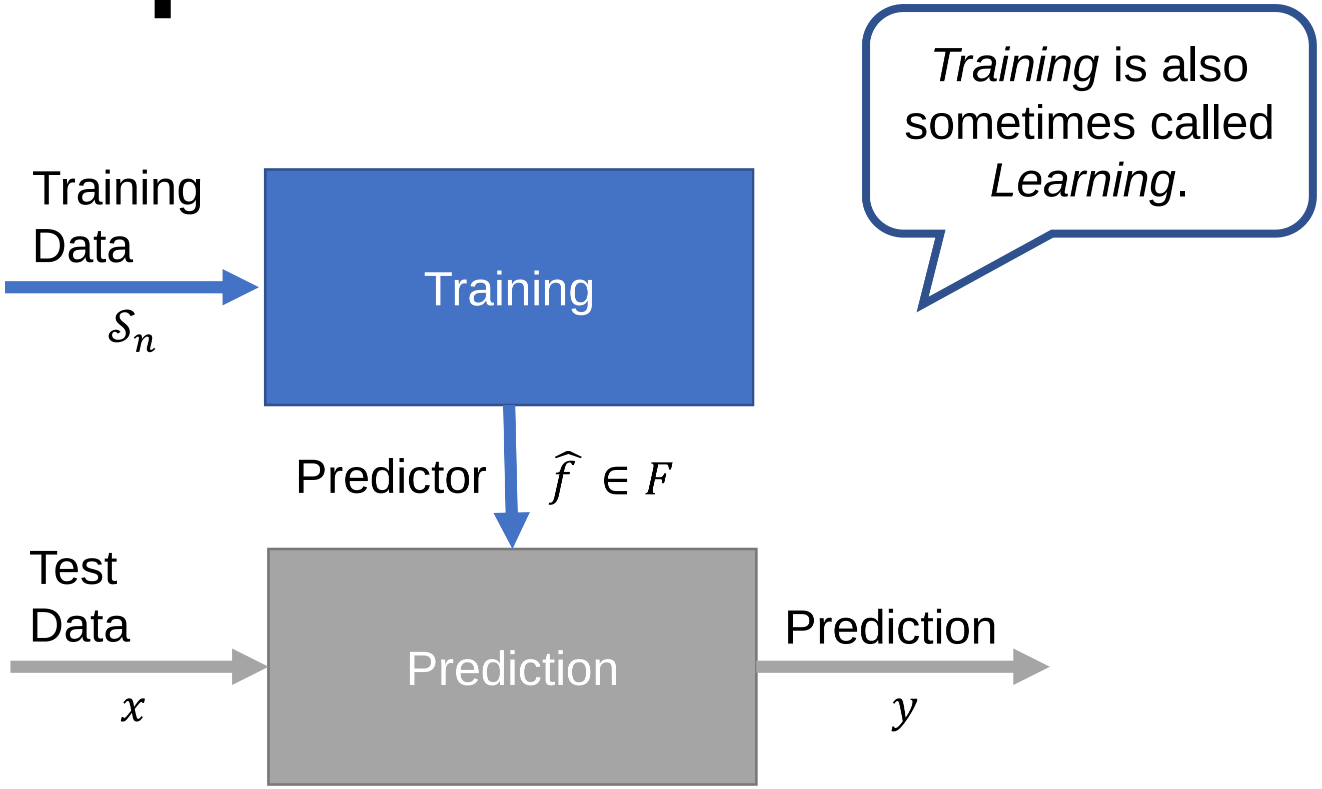
- **Empirical Risk and Least Squares Criterion**

Test Loss/Objective

$$R_{n'}^{test}(\theta) = \frac{1}{|Sn'|} \sum_{t=n+1}^{n+n'} (y^{(t)} - \theta \cdot x^{(t)})^2/2$$

Given a predictor $\hat{f}$, we use the test loss to measure how well it generalizes to new data.

Training and prediction



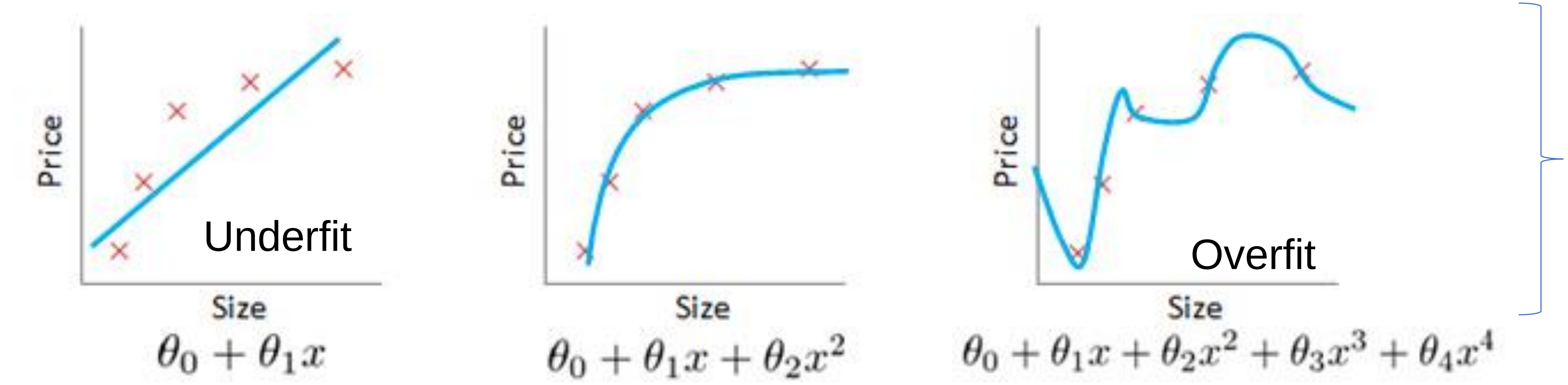
Assumption. Test data and training data are identically distributed.

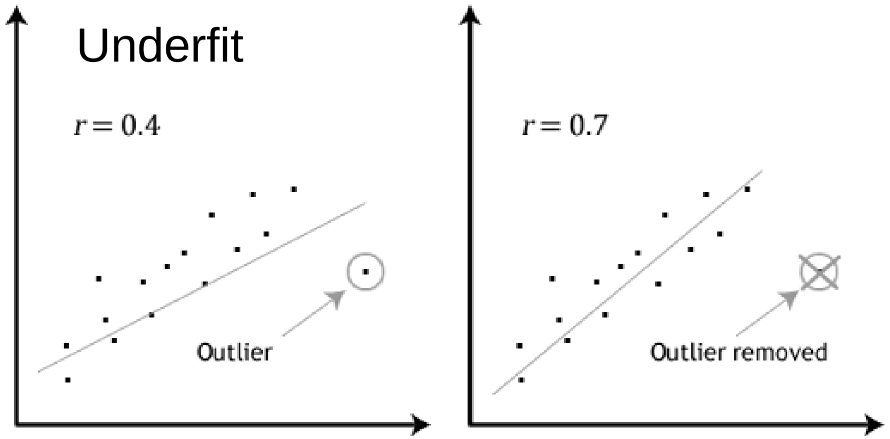
Generalization

The goal of machine learning is to find a predictor $\hat{f} \in F$ that generalizes well, i.e. that predicts well on test data $\mathcal{S}_{n'}$.

Under and Overfitting

$F =$





Model Selection

Overfitting. If model F is too big, then $\hat{f} \in F$ performs

- well on training data, but poorly on test data.

Underfitting. If model F is too small, then $\hat{f} \in F$ performs

- poorly on training data, and poorly on test data.

Finding a model with the right size is called model selection.

Optimization

Least Square Loss

Loss Function $\text{Loss}(z) = \frac{1}{2}z^2$

Squared error.
Penalize big errors more heavily.
CONVEX!!

Empirical Risk

$$R_1(\theta; x, y) = \text{Loss}\left(y^{(t)} - (\theta . x^{(t)})\right)$$

Point loss

$$R_n(\theta; \mathcal{S}_n) = \frac{1}{n}\sum_{(x,y)\in\mathcal{S}_n} R_1(\theta; x, y)$$

Average loss

$$= \frac{1}{n}\sum_{(x,y)\in\mathcal{S}_n} \frac{1}{2}\left(y^{(t)} - (\theta . x^{(t)})\right)^2$$

The training loss is the average of the point losses.

Risk = “Expected Loss”
Empirical = “of the Data”

Gradient Descent

- Use **gradient descent** to minimize $R_n(\theta)$

$$\nabla_\theta R_n(\theta) = \left[\frac{\partial R_n(\theta)}{\partial \theta_1}, \ldots, \frac{\partial R_n(\theta)}{\partial \theta_d}\right]^T$$

- Gradient points in the direction where $R_n(\theta)$ **increases**.
- Need to update the weight in the **opposite direction**.

$$\theta^{(k+1)} = \theta^{(k)} - \eta_k \nabla_\theta R_n(\theta)_{\theta=\theta^{(k)}}$$

Gradient Descent

- **Empirical Risk**

$$R_n(\theta) = \frac{1}{n}\sum_{t=1}^{n} \text{Loss}(y^{(t)} - \theta \cdot x^{(t)}) = \frac{1}{n}\sum_{t=1}^{n} (y^{(t)} - \theta \cdot x^{(t)})^2/2$$

- **Partial Derivative**

$$\nabla_\theta (y^{(t)} - \theta \cdot x^{(t)})^2/2 = (y^{(t)} - \theta \cdot x^{(t)})\nabla_\theta (y^{(t)} - \theta \cdot x^{(t)}) = -(y^{(t)} - \theta \cdot x^{(t)})x^{(t)}$$

- **Update of weight**

$$\theta^{(k+1)} = \theta^{(k)} - \eta_k \nabla_\theta R_n(\theta)_{\theta=\theta^{(k)}}$$

$$\theta^{(k+1)} = \theta^{(k)} + \eta_k (y^{(t)} - \theta \cdot x^{(t)})x^{(t)}$$

Stochastic Gradient Descent

1. Initialize the **weight** ($\theta^{(0)} = 0$).

2. Select $t \in \{1, \ldots, n\}$ at random

$$\theta^{(k+1)} = \theta^{(k)} + \eta_k (y^{(t)} - \theta \cdot x^{(t)}) x^{(t)}$$

3. Repeat Step (2) until stopping criterion is met.
(e.g. when improvement in $R_n(\theta)$ is small enough)

Closed Form Solution

- Minimize empirical risk directly by setting gradient to zero.

$$
\begin{aligned}
\nabla R_n(\theta)_{\theta=\hat{\theta}} &= \frac{1}{n}\sum_{t=1}^{n} \nabla_\theta \left\{ (y^{(t)} - \theta \cdot x^{(t)})^2/2 \right\}_{|\theta=\hat{\theta}} \\
&= \frac{1}{n}\sum_{t=1}^{n} \{ -(y^{(t)} - \hat{\theta} \cdot x^{(t)}) x^{(t)} \} \\
&= -\frac{1}{n}\sum_{t=1}^{n} y^{(t)} x^{(t)} + \frac{1}{n}\sum_{t=1}^{n} (\hat{\theta} \cdot x^{(t)}) x^{(t)} \\
&= \underbrace{-\frac{1}{n}\sum_{t=1}^{n} y^{(t)} x^{(t)}}_{=b} + \underbrace{\frac{1}{n}\sum_{t=1}^{n} x^{(t)} (x^{(t)})^T}_{=A} \hat{\theta} \\
&= -b + A\hat{\theta} = 0
\end{aligned}
$$

Closed Form Solution

- If A is invertible, we can find the weight as below

$$\hat{\theta} = A^{-1}b.$$

- Where, $b = \frac{1}{n}X^T\vec{y}, \quad A = \frac{1}{n}X^TX$

Regularization

RIDGE REGRESSION

Temp.
Weight Age on Mars

Height $y \approx \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_d x_d$

For simplicity, we ignore θ_0.

How do we ensure that $\theta_i = 0$ when feature x_i is irrelevant?

Pick simplest model that explains data ➔ **generalization**

RIDGE REGRESSION

Add a penalty.

Pressure to fit data

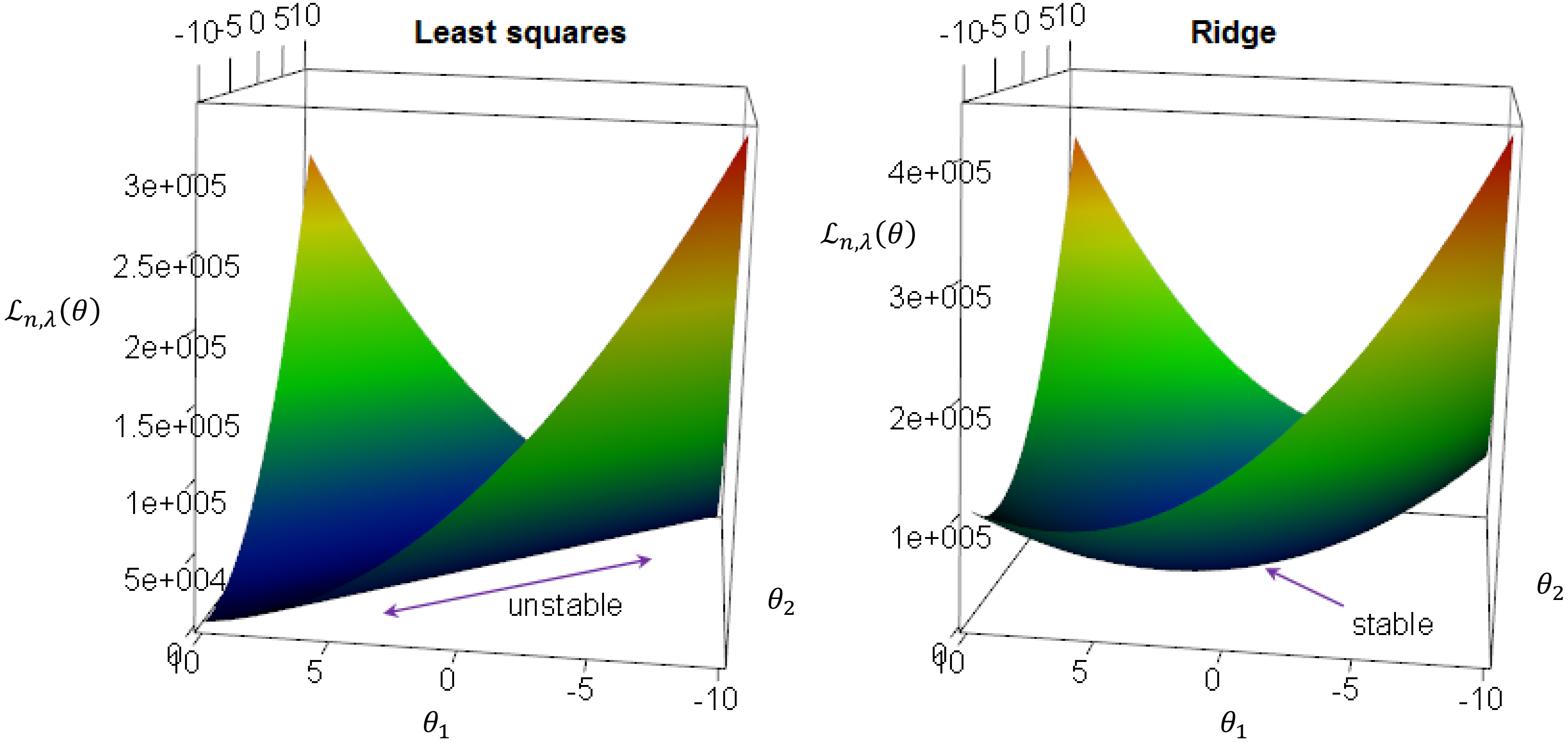
Pressure to simplify model

$$J_{n,\lambda}(\theta) = \frac{1}{n}\sum_{(x,y)\in\mathcal{S}_n} \frac{1}{2}(y - \theta^\top x)^2 + \frac{\lambda}{2}\|\theta\|^2$$

Regularization parameter $\lambda \geq 0$

Regularizer

RIDGE REGRESSION



TRAINING ALGORITHMS

Ridge Regression

$$J_{n,\lambda}(\theta) = \frac{1}{n}\sum_{(x,y)\in\mathcal{S}_n} \frac{1}{2}(y - \theta^\top x)^2 + \frac{\lambda}{2}\|\theta\|^2$$

Gradient

$$\nabla J_{n,\lambda}(\theta) = \nabla_\theta \left\{\frac{\lambda}{2}\|\theta\|^2 + (y^{(t)} - \theta \cdot x^{(t)})^2/2\right\}_{|\theta=\theta^{(k)}}$$

$$\nabla J_{n,\lambda}(\theta) = \lambda\theta^{(k)} - (y^{(t)} - \theta^{(k)} \cdot x^{(t)})x^{(t)}$$

Gradient Descent

$$\theta^{(k+1)} = (1 - \lambda\eta_k)\theta^{(k)} + \eta_k(y^{(t)} - \theta \cdot x^{(t)})x^{(t)}$$

Without regularization, i.e. $\lambda = 0$, this shrinkage factor equals 1.

TRAINING ALGORITHMS

Ridge Regression

$$J_{n,\lambda}(\theta) = \frac{1}{n} \sum_{(x,y)\in \mathcal{S}_n} \frac{1}{2}(y - \theta^\top x)^2 + \frac{\lambda}{2}\|\theta\|^2$$

Gradient

$$\nabla J_{n,\lambda}(\theta) = \lambda\theta + \frac{1}{n}(X^\top X)\theta - \frac{1}{n}X^\top Y$$

Exact Solution

$$\nabla J_{n,\lambda}(\hat{\theta}) = 0 \quad \Leftrightarrow \quad \lambda\hat{\theta} + \frac{1}{n}(X^\top X)\,\hat{\theta} = \frac{1}{n}X^\top Y$$

$$\Leftrightarrow \quad \hat{\theta} = (n\lambda I + X^\top X)^{-1} X^\top Y$$

This matrix is always invertible when $\lambda > 0$.

TRAINING LOSS VS TEST LOSS

Training Loss

$$J_{n,\lambda}(\theta;\mathcal{S}_n) = \frac{1}{n}\sum_{\boxed{(x,y)\in\mathcal{S}_n}} \frac{1}{2}(y-\theta^\top x)^2 + \boxed{\frac{\lambda}{2}\|\theta\|^2}$$

Test Loss/Error

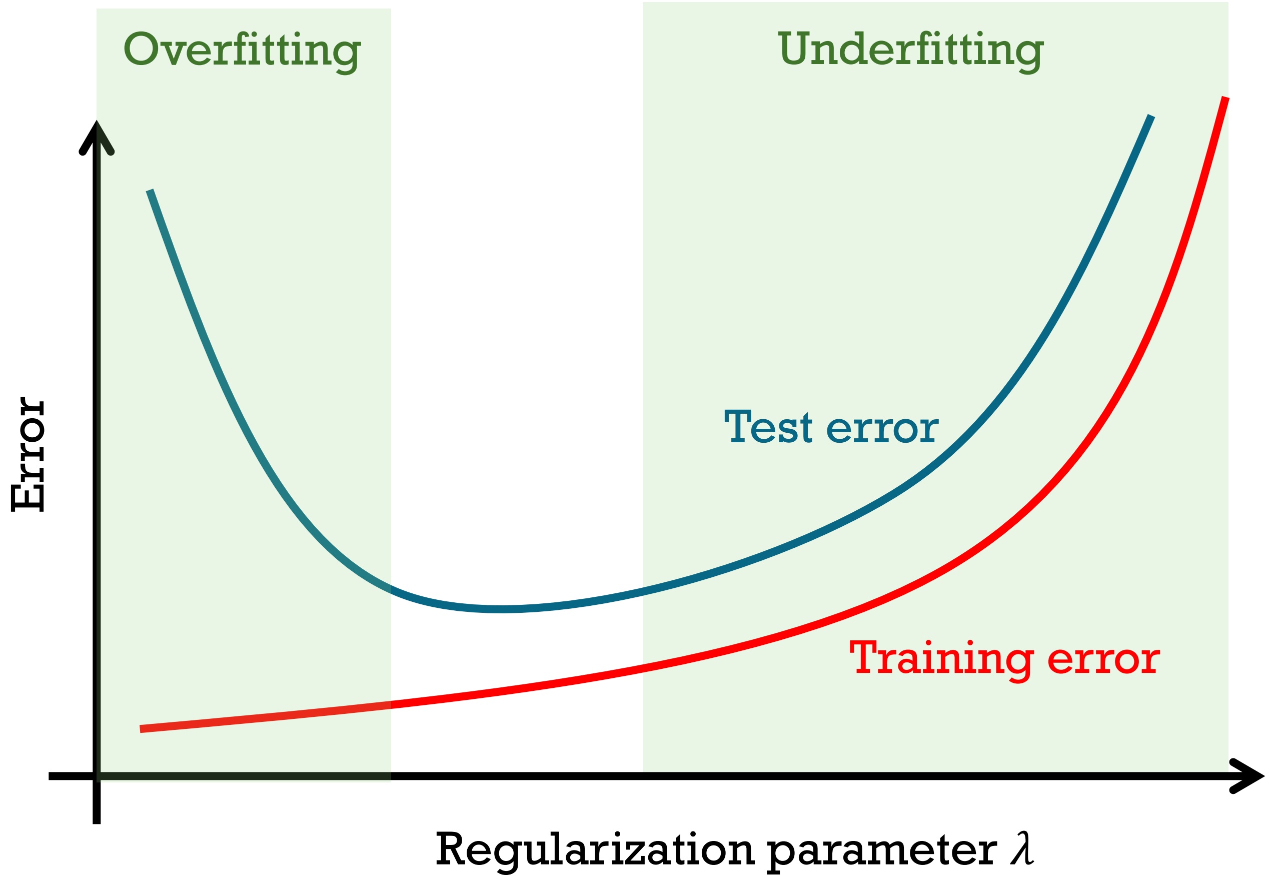
$$\mathcal{R}(\hat{\theta};\mathcal{S}_{n'}) = \frac{1}{|s_{n'}|}\sum_{\boxed{(x,y)\in\mathcal{S}_{n'}}} \frac{1}{2}\left(y-\hat{\theta}^\top x\right)^2$$

Training Error

$$\mathcal{R}(\hat{\theta};\mathcal{S}_n) = \frac{1}{n}\sum_{\boxed{(x,y)\in\mathcal{S}_n}} \frac{1}{2}\left(y-\hat{\theta}^\top x\right)^2$$

The *training error* is the test loss applied to the training set, and it may be different from the training loss.

EFFECT OF REGULARIZATION



PICKING HYPERPARAMETERS

- The regularization parameter λ is an example of a *hyperparameter*, which affects the model complexity.

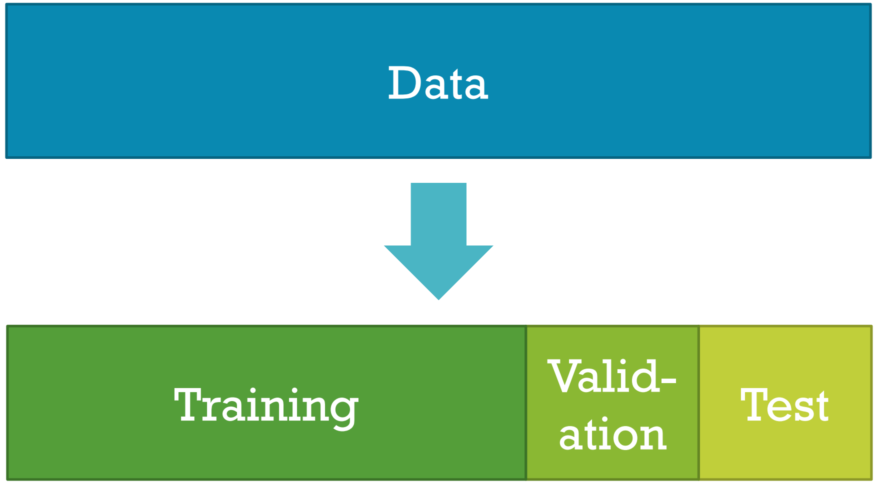
- We don't usually have access to the test data.
  How do we know if the value of λ minimizes the test loss?

- The solution is to create a *validation* data set, as a proxy to the test data, and to compute the *validation loss*.

VALIDATION SET

Split the data into

- **Test set** $\mathcal{S}_{n'}$
  For evaluating, reporting performance at the end
- **Training set** $\mathcal{S}_n$
  For training optimal parameters in a model
- **Validation set** $\mathcal{S}_{\text{val}}$
  For model selection, e.g. picking λ in ridge regression. Acts as a proxy for test set.



VALIDATION LOSS

The *validation loss* is the test loss applied to the validation set.

Example. Ridge Regression

Test loss/error $\mathcal{R}\left(\hat{\theta}; \mathcal{S}_{n'}\right) = \frac{1}{n} \sum_{(x,y) \in \mathcal{S}_{n'}} \frac{1}{2} \left(y - \hat{\theta}^\top x\right)^2$

Validation loss/error $\mathcal{R}\left(\hat{\theta}; \mathcal{S}_{\mathrm{val}}\right) = \frac{1}{|s_{val}|} \sum_{(x,y) \in \mathcal{S}_{\mathrm{val}}} \frac{1}{2} \left(y - \hat{\theta}^\top x\right)^2$

MODEL SELECTION