Supervised Machine Learning

Linear Regression

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Outline

1. Introduction

2. Supervised Linear Model

3. Use Case

4. Model Assessment

5. References

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1. **Introduction**
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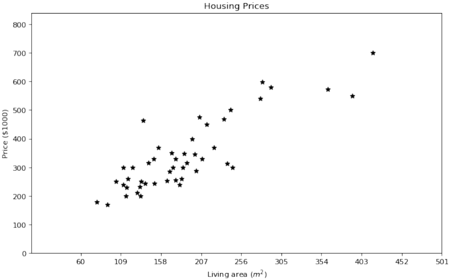
House price prediction

Dataset of housing prices

Living area (m^2)	Price ($1000)
196	400
149	330
223	369
132	232
279	540
⋮	⋮



Outline

1 Introduction

2 Supervised Linear Model
- Linear regression
- Cost function
- Least mean squares algorithm
- Gradient descent algorithm

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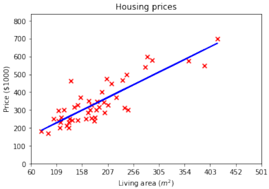
Why do we need to study supervised linear models?

- Linear model provides an introduction to **core concepts** of machine learning
- It may be employed for a variety of reasons:
  1. to produce a so-called trend line (or curve) that can be used to help visually summarize
  2. drive home a particular point about the data under study
  3. learn a model so that precise predictions can be made regarding output values in the future
- Many real process can be **approximated** with linear models
- Linear regression usually appears as a **module** of large systems
- Linear problems can be analyzed **analytically**

Variable types and terminology

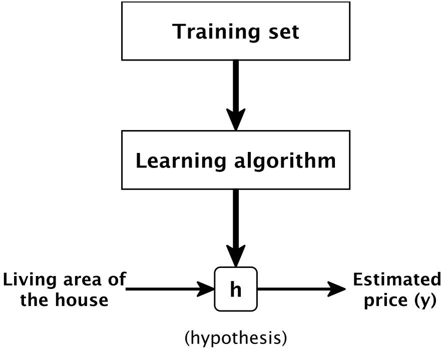
- An **input variable** also called **feature** is denoted by $x^{(i)}$
- $y^{(i)}$ denotes an **output** or **target** variable
- A pair $(x^{(i)}, y^{(i)})$ is called a **training sample**
- $(x^{(i)}, y^{(i)}); i = 1, \dots m$ denotes the **training set**
- $\mathcal{X} \in \mathbb{R}$ denotes the space of input values, and $\mathcal{Y} \in \mathbb{R}$ denotes the space of output values

Stating the learning task



Learning task

- Given the value of an input vector $\mathcal{X}$, make a good prediction of the output $\mathcal{Y}$, denoted by $\hat{Y}$. If $\mathcal{Y}$ takes values in $\mathbb{R}$, then so should $\hat{\mathcal{Y}}$
- Assuming that we have a training set $(x^{(i)}, y^{(i)})$ or $(x^{(i)}, g^{(i)})$, $i = 1, \dots, m$, where each input $x^{(i)} \in \mathbb{R}$ is column vector.
- The goal of **supervised learning** models comprises in giving the "right answer" for each example in the data
- Regression models aim to **predict real-valued outputs**



Training set

Learning algorithm

Living area of the house

h

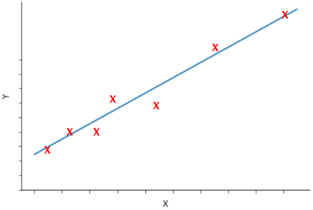
Estimated price (y)

(hypothesis)

h maps x's to y's

- **How do we represent h?**

$$h_\theta(x) = \theta_0 + \theta_1 x$$



- Linear regression with one variable
- **Univariate** linear regression

Linear regression

- $h : \mathcal{X} \rightarrow y$ is a linear combination of the input variables

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n = \theta_0 + \sum_{i=1}^{n} \theta_i x_i$$

- where,
  - $\theta_0, \theta_1, \ldots, \theta_n$ are the **parameters** (i.e., weights) of the model
  - θ_0 is the **intercept**, also known as **bias** or **offset** in machine learning
  - We assume that x_1 = 1 and thus, we include θ_0 in the coefficients θ. Thus

$$h_\theta(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x$$

  - θ and x are both vectors
  - n is the number of variables

Cost function

Training set

Living area (m^2)	Price (\$1000)
196	400
149	330
223	369
132	232
279	540
$\vdots$	$\vdots$

- Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x$
- How to choose $\theta_i' s?$
    - Make $h(x)$ as close as possible to y
- A **cost function** measures how close the $h(x^i)$ are to the true value of y^i

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} \left(h_\theta(x^i) - y^i\right)^2$$

- Least-squares cost function that leads to the **ordinary least squares** regression model

Cost function: intuition

- **Hypothesis**:

  $$h_\theta(x) = \theta_0 + \theta_1 x$$

- **Parameters**:

  $$\theta_0, \theta_1$$

- **Cost function**:

  $$J(\theta_0, \theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta x^{(i)} - y^{(i)}\right)^2$$

- **Goal**:

  $$\underset{\theta_0,\theta_1}{\text{minimize}}\, J(\theta_0, \theta_1)$$

Simplified

- **Hypothesis**:

  $$h_\theta(x) = \theta_1 x$$

- **Parameters**:

  $$\theta_1$$

- **Cost function**:

  $$J(\theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta x^{(i)} - y^{(i)}\right)^2$$

Goal:

$$\underset{\theta_1}{\text{minimize}}\, J(\theta_1)$$

Least mean squares (LMS) algorithm

- **Coast function**:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^i) - y^i\right)^2$$

- **Goal**: **Goal**:

$$\underset{\theta}{\text{minimize}}\, J(\theta)$$

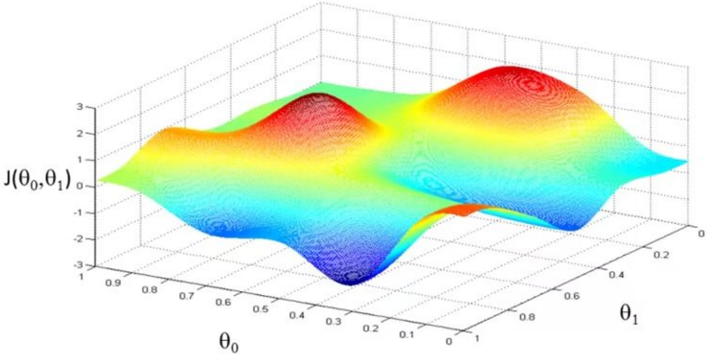
- Search algorithm that:
  1. Starts with an initial guess for θ
  2. Repeatedly changes θ to make $J(\theta)$ smaller until converge to a value of θ that minimizes $J(\theta)$

- **Gradient descent algorithm**:
  1. starts with some initial θ
  2. repeatedly updates θ:

$$\theta_j = \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta) \;\; \forall\, j = 0, \;\cdots, n$$

  3. where α is called the **learning rate**

Gradient descent algorithm



Dealing with only one training example

repeat until `convergence` {

$$\theta_j = \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$$

(for j = 0 and j = 1)

}

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} \left(h_\theta(x) - y\right)^2 \\
&= 2 \cdot \frac{1}{2} \left(h_\theta(x) - y\right) \cdot \frac{\partial}{\partial \theta_j} \left(h_\theta(x) - y\right) \\
&= \left(h_\theta(x) - y\right) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y\right) \\
&= \left(h_\theta(x) - y\right) x_j
\end{aligned}$$

This gives the update rule:

$$\theta_j = \theta_j + \alpha(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)}$$

Batch gradient descent

- Each step of gradient descent uses all the training examples
- Stochastic gradient descent
- Mini-batch gradient descent

Batch gradient descent

repeat until `convergence` {

$$\left.\begin{aligned} \theta_0 &:= \theta_0 - \alpha \tfrac{1}{m} \textstyle\sum_{i=1}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right) \\ \theta_1 &:= \theta_1 - \alpha \tfrac{1}{m} \textstyle\sum_{i=1}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right) x^{(i)} \end{aligned}\right\} \begin{array}{l}\text{update } \theta_0 \text{ and } \theta_1 \\ \text{simultaneously}\end{array}$$

}

Mini-batch gradient descent

- Each step of gradient descent uses b training examples
- For instance, $b = 10$ and $m = 1000$

```
repeat until convergence {
  for $i = 1, 11, 21, \ldots, 991$ {
    $\theta_0 = \theta_0 - \alpha \frac{1}{10} \sum_{i=k}^{i+9} (h_\theta(x^{(i)}) - y^{(i)})$
    $\theta_1 = \theta_1 - \alpha \frac{1}{10} \sum_{i=k}^{i+9} (h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}$
}
```

Stochastic gradient descent

Each step of gradient descent uses one training example

```
repeat until convergence {
    for $i = 1, \ldots, m$ {
        $\theta_j = \theta_j - \alpha(y^{(i)} - h_\theta(x^{(i)}))x^{(i)}$   (for every j)
    }
}
```

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Exploring the Boston housing dataset

- We will explore the Housing dataset, which contains information about houses in the suburbs of Boston
- It was collect by Harrison Jr and Rubinfeld[1] in 1978
- The Housing Dataset has been made freely available and it can be download from the UCI machine learning repository at *archive.ics.uci.edu/ml/machine-learning-databases/housing*
- It comprises 506 samples and 13 features. Thus, the goal is to predict the price of the houses using the given features

[1] David Harrison Jr and Daniel L Rubinfeld. "Hedonic housing prices and the demand for clean air". In: *Journal of environmental economics and management* 5.1 (1978), pp. 81–102.

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4 **Model Assessment**
- Learning Curves
- Model Complexity & Generalization
- Regularization
- Validation & Cross-Validation

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Assessing regression model performance

- **Residual sum of squares (RSS)**

$$RSS = \sum_{i=1}^{n} \left(y_i - f(x^i)\right)^2$$

- **Root-mean squared error (RMSE)**

$$RMSE = \sqrt{\frac{\sum\limits_{i=1}^{n} \left(y_i - f(x^i)\right)^2}{n}}$$

- **Relative squared error (RSE)**

$$RSE = \frac{\sum\limits_{i=1}^{n} \left(y_i - f(x^i)\right)^2}{\sum\limits_{i=1}^{n} \left(y^i - \bar{y}\right)^2}$$

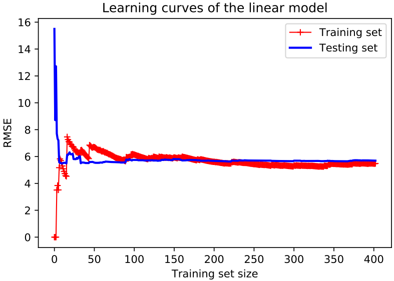
- **Coefficient of determination**

$$R^2 = 1 - RSE$$

Learning curves

- When building a data model, our goal is to design one that better fits the data
- How to assess that we are building a good enough model?
- In other words, what can we do to check that the model is not **overfitting** or **underfitting** the data?
- A model is **overfitting** when it performs well on training data, but generalizes poorly on test data
- A model is **underfitting** when it performs poorly on both training and test sets
- We can use **learning curves** to visualize the performance of a model on training and test sets as a function of the training size
    - To generate them, we have to train the model on different sized sets

Example of learning curves



- When a model is **underfitting** the training data, adding more training example is **useless.** We must use a more complex model or come up with better features
- On the other hand, when a model is **overfitting**, we can feed it more training examples until the validation error reaches the training error

Bias, variance, and trade-off

- A model generalization error can be expressed as the sum of its bias, variance, and irreducible error
- **Bias** comprises the wrong hypotheses, such as assuming that the data follow a linear law. A high-biased model is most likely to underfit the training data
- **Variance** comprises excessive sensitivity for small variations in the training data. A model with high-degree of freedom usually has high-variance, and thus is most likely to overfit the training data.
- **irreducible error** comprise the noises of the data. One way to reduce this part of the generalization error is to clean up the data.
- **Trade-off**:
  - `increasing a model's complexity` commonly `increases` its variance and `reduces` its `bias`
  - `Reducing a model's complexity` increases its `bias` and `reduces` its `variance`

How to define learning in machine learning?

- Several questions arise when designing and analyzing algorithms that learn from data. Examples of questions include:
  1. What can be learned efficiently?
  2. What is inherently hard to learn?
  3. How many examples are needed to learn successfully?
  4. Is there a general model of learning?
- The **Probably Approximately Correct (PAC)** learning framework helps defines the class of learnable concepts in terms of **number of sample points** needed to achieve an approximate solution, **sample complexity**, and the time and space complexity of a learning algorithm.

How to assess learning in machine learning?

- Let us denote $\mathcal{X}$ the set of all possible examples, $\mathcal{Y}$ the set of all possible label or target values, and that $\mathcal{Y} = \{0, 1\}$
- A concept $c : \mathcal{X} \mapsto \mathcal{Y}$ is a mapping from $\mathcal{X}$ to $\mathcal{Y}$.
- $\mathcal{C}$ is a concept class that comprises the concepts we may wish to learn
- The **learning problem** can be formulated as follows:
  - The learner considers a fixed set of all possible concepts $\mathcal{H}$, called *hypothesis set*, with input sample $\mathcal{S} = (x^i, \ldots, x^p)$ draw i.i.d according to $\mathcal{D}$ as well as the labels $c(x_i), \ldots, c(x^p)$ with $c \in \mathcal{C}$
  - The task comprise in using the labeled sample $\mathcal{S}$ to select a hypothesis $h_s \in \mathcal{X}$ that as a small **generalization error** with respect to c.
- The generalization error of a hypothesis $h \in \mathcal{H}$ is also known as the **risk** or **true error**.

Generalization error

Given a hypothesis $h \in \mathcal{H}$, a target concept $c \in \mathcal{C}$, and an underlying distribution $\mathcal{D}$, the generalization error or risk of h is defined by

$$R(h) = \underset{x \sim \mathcal{D}}{\mathbb{P}}[h(x) \neq c(x)] = \underset{x \sim \mathcal{D}}{\mathbb{E}}[1_{h(x) \neq c(x)}]$$

- Since both the distribution $\mathcal{D}$ and the target concept c is unknown, a learner cannot direct access the generalization error. It can only measure the **empirical error** of a $h \in \mathcal{H}$ on the labeled sample $\mathcal{S}$

Empirical error

Empirical error

- Given a hypothesis $h \in \mathcal{H}$, a target concept $c \in \mathcal{C}$, and a sample $S = (x^i, \ldots, x^n)$, the empirical error or empirical risk of h is defined by

$$\hat{R}_s(h) = \frac{1}{n} \sum_{i=1}^{n} 1_{h(x_i) \neq c(x_i)}$$

- The **empirical error** of $h \in \mathcal{H}$ is its average error over the sample S, while the **generalization error** is its expected error based on the distribution $\mathcal{D}$

PAC-Learning

PAC-learning

- A concept class $\mathcal{C}$ is said to be PAC-learnable if there exists an algorithm $\mathcal{A}$ and a polynomial function $poly(.,.,.,.)$ such that for any $\epsilon > 0$ and $\delta > 0$, for all distributions $\mathcal{D}$ on $\mathcal{X}$ and for any target concept $c \in \mathcal{C}$, the following holds for any sample size $m \geq poly(\frac{1}{\epsilon}, \frac{1}{\delta}, n, size(c))$

$$\underset{S \sim \mathcal{D}^m}{\mathbb{P}}[R(h_s) \leq \epsilon] \geq 1 - \delta$$

- if $\mathcal{A}$ further runs in $poly(\frac{1}{\epsilon}, \frac{1}{\delta}, n, size(c))$, the $\mathcal{C}$ is considered to be efficiently PAC-learnable.
- When such $\mathcal{A}$ exists, it is called a *PAC-learning algorithm* for $\mathcal{C}$
- The parameter $\delta > 0$ defines the confidence interval $1 - \epsilon$ and $\epsilon > 0$ the accuracy $1 - \epsilon$.

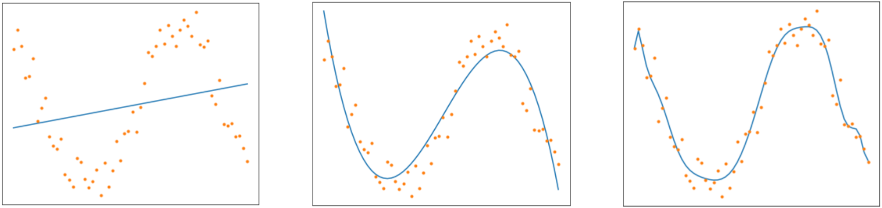
Learning comprises generalization

- Machine learning is fundamentally about **generalization**
- The problem comprises in selecting a function out of a *hypothesis set*, that is a subset of the family of all functions
- The selected function is subsequently used to label all instances, including **unseen** examples
- How should a hypothesis set be chosen?
  - With a rich or complex hypothesis set, the learner may choose a predictor that is consistent with the training set
  - With a less complex one, it may have unavoidable errors on the training set
- Which one will lead to a better **generalization**?
- How should we define the complexity of a hypothesis set?

What is generalization?

- *It is the ability of a model to adapt properly to* ***unseen data*** *drawn from the same distribution as the one used to create the model*
- Data are noisy, for different reasons
  1. errors during the acquisition phase
  2. errors in labeling the data points
  3. hidden or latent features
- We learn f by minimizing some variant of empirical risk, what can you say about the true risk?
- Two factors determine generalization ability:
  1. model complexity
  2. training set size

Understanding overfitting & underfitting



$\beta_0 + \beta_1 x$

$\beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

$\beta_0 + \beta_1 x + \cdots + \beta_{15} x^{15}$

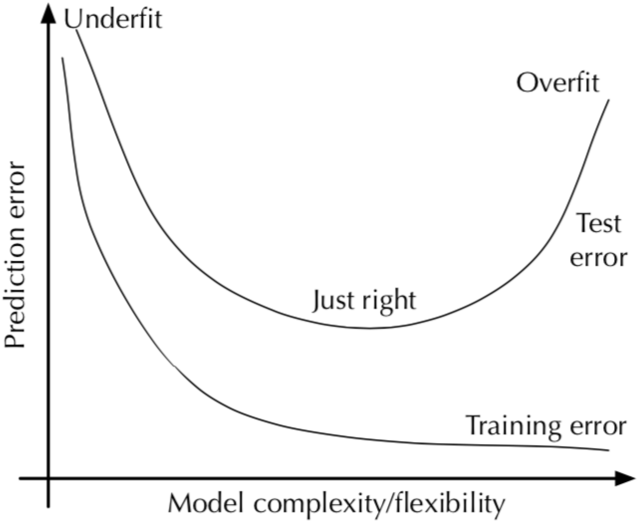
Underfitting $\mapsto$ **“high bias”**

“Just right”

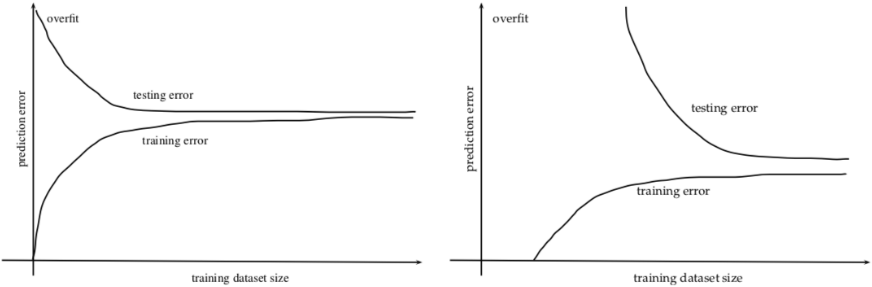
“overfitting” $\mapsto$ **“high variance”**

- In the **Overfitting** scenario, the learned hypothesis may fit the training set very well, but fail, but fail to **generalize** to new examples
  - It is usually caused by complicated function that creates various unnecessary curves and angles unrelated to the data
  - It has a large estimation error
- **Underfitting or high bias** occurs when the hypothesis function maps poorly to the trend of the data
  - It is usually caused by a function that is very simple or that uses only few features
  - It has a large approximate error

Generalization error vs. model complexity trade-off



Fixed model complexity vs. dataset size



Bias vs. variance trade-off

- **Bias** is the difference between the expected value of the estimator and the real value predicted by the estimator

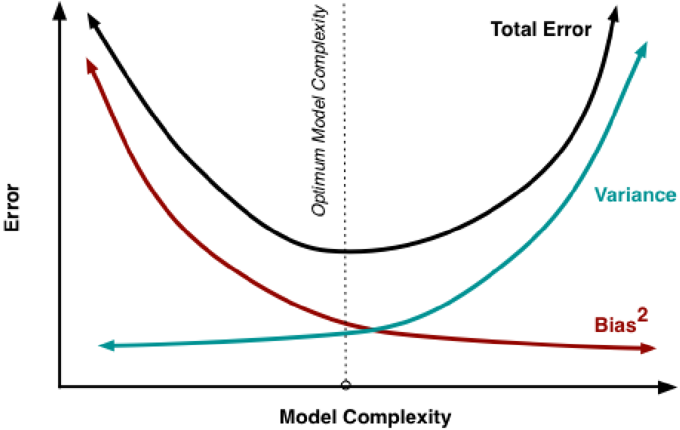
$$Bias(f(x)) = \mathbb{E}[f(x) - y]$$

  - A simple model has a high bias
  - High bias can lead to **underfitting**
- **Variance** is the deviation from the expected value of the estimates

$$Var(f(x)) = \mathbb{E}[(f(x) - \mathbb{E}(f(x)))^2]$$

  - A complex model has a high variance
  - High variance usually leads to **overfitting**

Bias vs. variance trade-off



Addressing overfitting

1. Reduce the number of features
    - Manually select which feature to keep
    - Model selection algorithm
2. Regularization
    - Keeps all the features, but reduce the magnitude of the parameters
    - It works when there are many features contributing to predict y

Supervised learning assumption

- **Training set** $\mathcal{D} = \{x^i, y^i\}_{i=1..n}$
- **Regression** $y^i \in \mathbb{R}$
- **Classification** $y^i \in \{0, 1\}$
- **Goal**: find a function f on the training set such that $f(x^i) \approx y^i$
- **Empirical error** of f on the training set, given a loss function $\mathcal{L}$

$$\mathbb{E}(f|\mathcal{D}) = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(y^i, f(x^i))$$

  - **Regression**

$$\mathcal{L}(y^i, f(x^i)) = (y^i - f(x^i))^2$$

  - **Classification**

$$\mathcal{L}(y^i, f(x^i)) = 1_{y^i \neq f(x^i)}$$

Empirical error

- On the training set, it is a poor estimate of the **generalization error**
- If the model is overfitting, the generalization error can be arbitrarily large
- Our goal is to estimate the generalization error on unseen data, which we might not have

Complex learning models may lead to unstable behavior

- Complex learning algorithms can become **unstable**; i.e., highly dependent of the training data
- Instability is a manifestation of a tendency to overfit
- **Regularization** is a general method to avoid such overfitting by applying additional constraints to the weights vector
- A common strategy is to make sure that the weight are, on average, small in magnitude, which is known as **shrinkage**

Unstable learning algorithm tends to overfit

- A regularization function measures the complexity of the hypotheses
- It can be also seen as a **stabilizer** of the learning algorithm
- An algorithm is considered **stable** if a **slight change** of its input **does not change** its **output too much**
- Let A be a learning algorithm, $S = (z_i, \ldots, z_m)$ be a training set of m examples and $A(S)$ denote the output of A
- We can say that algorithm A is suffering from overfitting if the difference between the true risk of its output $L_d(A(S))$, and the empirical risk of its output $L_s(A(S))$ is large.
- Thus, our interest is in the expectation

$$\mathbb{E}_s[L_{\mathfrak{D}}(A(S)) - L_s(A(S))$$

Unstable learning algorithm tends to overfit

- In this case, stability can be defines as:
  - let z' be an additional example
  - $S^{(i)}$ be the training set obtained by replacing the i^{th} example of S

$$S^{(i)} = (z_i, \ldots, z_{i-1}, z', z_{i+1}, \ldots, z_m)$$

- Stability measures the effect of the small change of the input on the output of A by comparing the loss of the hypotheses $A(S)$ on z_i to the loss of the hypotheses $A(S(^{(i)}))$ on z_i.
- A good learning algorithm will have $\ell(A(S^{(i)}), z_i) - \ell(A(S), z_i) \geq 0$, since in the first term the learning algorithm does not observe the example z_i while in the second the term z_i is indeed observed
- If the difference is very large, the learning algorithm might been overfitting
- Examples of regularized linear models include: **Rigde Regression**, **Lasso Regression**, and **Elastic Net**

Ridge regression

- It adds a regularization term $\alpha \sum_{i=1}^{n} \theta_i^2$ to the cost function
- The regularization term α forces the learning model to not only fit the data but also to keep the weights of the model as small as possible
- The regularization term α is only used during the training phase
- In this case, the regularization term α is a hyperparameter that controls how much the want to regularize the model
  - When $\alpha = 0$, ridge regression is just a linear regression model
  - When α is a large value, all the weights end up close to zero, and the result is a flat line going through the data's mean
- Cost function:

$$J(\theta) = MSE(\theta) + \alpha \frac{1}{2} \sum_{i=1}^{n} \theta_i$$

Ridge Regression

- It is based on sum of squared residuals penalty

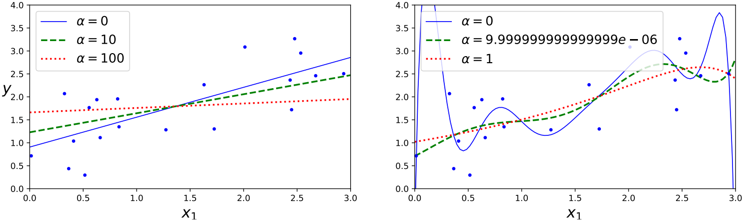
$$\hat{\theta}_{ridge} = \underset{\theta}{\operatorname{argmin}}\, (y - X\theta)^T (y - X\theta) + \alpha ||\theta||^2$$

- where $||\theta||^2 = \sum_{i=1}^{p} \theta_i^2$ is the squared norm of the vector θ, or equivalently the dot product $\theta^T\theta$
- α is a scalar determining the amount of the regularization
- Its closed-form can be written as:

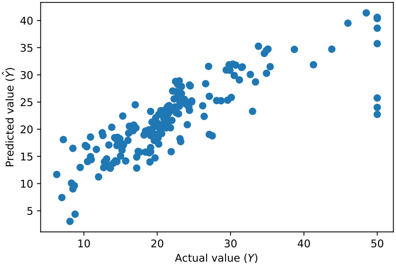
$$\hat{\theta} = (X^T X + \alpha I)^{-1} X^T y$$

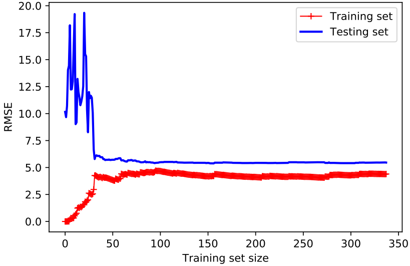
- Ridge regression shrinks the coefficients towards 0, but does not lead to a **sparse model**

Ridge regression: example with simulated data



Ridge regression: predicting Boston housing price





Lasso regression

- Least absolute shrinkage and selection operator regression method adds a regularization term to the cost function
- It uses the l_1 norm of the weights vector instead of the half square of the l_2 norm

$$J(\theta) = MSE(\theta) = \alpha \sum_{1}^{n} |\theta_i|$$

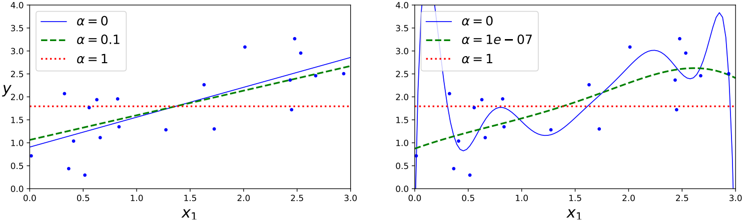
- An important characteristics of Lasso is that it tends to completely remove the weights of the least important features
- It means that Lasso regression automatically perform `feature selection`

Lasso

$$\hat{\theta}_{lasso} = \underset{\theta}{\operatorname{argmin}} ||y - \theta||_2^2 + \alpha||\theta||_1$$

- It stands for *Least absolute shrinkage and selection operator*
- It replaces the ridge regularization term $\sum_{i=1}^{n} \theta_i^2$ with the sum of the absolute weights $\sum_{i=1}^{n} |\theta_i|$
- Lasso regression favors sparse solutions
- It is quite sensitive to the regularization parameter α
- There is no closed form solution and numerical optimization technique must be applied

Lasso regression: example



In summary

- Ridge regression
  - correlated variables get similar weights
  - identical variables get identical weights
  - It is not sparse
- Lasso
  - correlated variables are randomly picked out
  - It is sparse

Elastic Net

- The regularization term is a mix of both Ridge and Lasso' regularization terms, and it controls the mix ratio r
  - When $r = 0$, Elastic Net is similar to Ridge regression
  - When $r = 1$, it is equivalent to Lasso regression
- Cost function

$$J(\theta) = MSE(\theta) + r\alpha \sum_{i=1}^{n} |\theta_i| + \frac{1-r}{2}\alpha \sum_{i=1}^{n} \theta_i^2$$

When should we use Linear Regression, Ridge, Lasso, or Elastic Net?

- It is almost a good choice to implement some regularization
- **Ridge** regression is usually good default option
- **Lasso** or **Elastic Net** should be preferred when observed that only few features are useful, since they tend to remove useless features' weights
- In general, **Elastic Net** is preferred over **Lasso** as **Lasso** may behave incorrectly when the number of features is greater than the number of training instances or when many features are correlated

Empirical vs. true risk

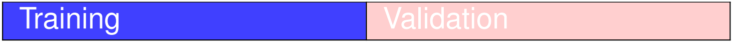
- In general, it is defined by

$$R(f) = R^{emp} + \text{overfit penalty}$$

- Overfit penalty depends on the complexity of the model
- **Regularization** approximates the overfit penalty. When the complexity of the model increases, we set up a larger overfit penalty
- **Cross-validation** tries to estimate $R(f)$ directly

Holdout method

- **Holdout method** is a popular approach for estimating the generalization performance of machine learning models
- Using **holdout method**, we split the initial dataset into training and test sets



- We want to choose a model that performs best on a **validation set** independent of the **training set**
- Since we have not used the validation data during the training phase, the validation set can be considered **unseen data**
- In this case, the error on the validation set is an estimation of the generalization error
- What is another issue in this approach?

Model selection is a classification problem

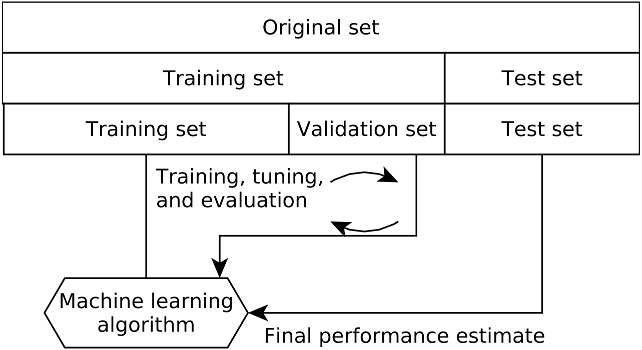
- We are interested in tuning and comparing different parameter settings to further improve the performance, for making prediction on unseen data
- This process is called **model selection**
- Model selection refers to a given classification problem for which we want to select the optimal values of tuning parameters
- Therefore, if we reuse the same dataset over and over again during model selection, it will become part of our training data and thus the model will be more likely to overfit

Dealing with multiple models

- What should we do if we want to choose among k different models?
  1. We have to train each model on the training set
  2. Then, compute the prediction error of each model on the validation set
  3. Finally, select the model with the smallest prediction error on the validation set
- In that case, what will be the generalization error?
  - It is hard to say
  - Validation data was used to select the model
  - Actually, as we have looked at the validation data, it is not anymore a good proxy for unseen data

Holdout cross-validation

- A better way of using the holdout method for method selection comprises in splitting the dataset into three parts: a training set, a validation set, and a test set



Original set

Training set | Test set

Training set | Validation set | Test set

Training, tuning, and evaluation

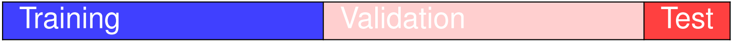
Machine learning algorithm

Final performance estimate

- Therefore, the estimation error is sensitive to how we partition the training and the validation sets

Handling the problem of validation set

- We have to set aside a test set that remains untouched during the training and the validation phases
- With the test set, we can use it to estimate the generalization error


Training
Validation
Test

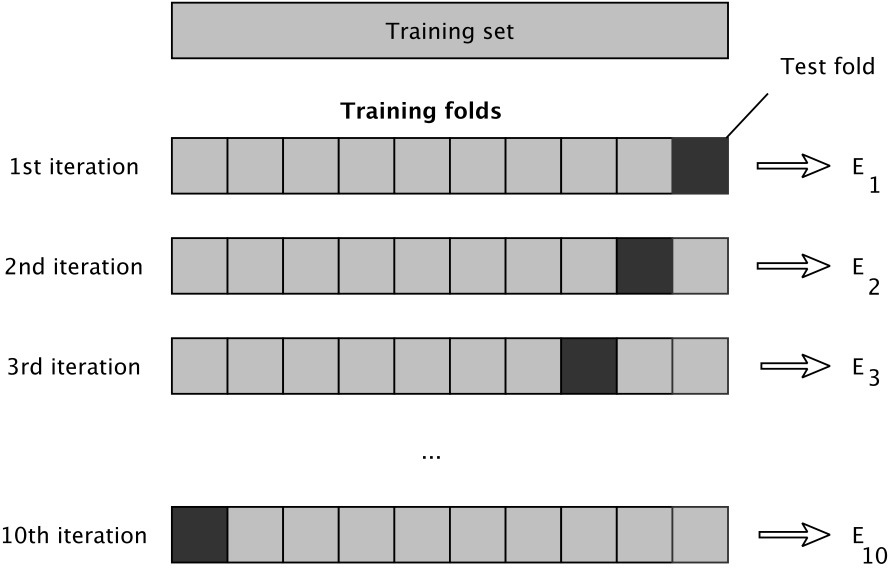
- How we decide the size of the training, validation, and test sets?
- How do we know that we have enough data to evaluate the prediction and the generalization errors?
- In **model selection**, we aim to pick the best model
- Whereas, in **model assessment**, we want to estimate the prediction errors on unseen data

We can use **cross-validation** and **bootstrap** techniques to empirically evaluate our model

K-fold cross-validation

- **k-fold cross-validation** is a technique designed to give an accurate estimate of the true error without “wasting” too much data
- In the k-fold cross-validation, the original training set is partitioned into k folds without replacement
- $k-1$ folds are used for the model training and one fold is used for testing
- For each fold, the model is estimated on the union of the other folds and then, the error of its output is estimated using the fold
- The average of all the errors is the estimate of the true error
- Once the best parameter is chosen, the model is retrained using the parameters of the entire training set

K-fold cross-validation



K-fold cross-validation algorithm

```
Input:
  training set $S = (x^1, y^i), \ldots, (x^p, y^p)$
  set of parameter values $\Theta$
  learning algorithm $\mathcal{A}$
  $k$ (number of folds)
split $S$ into $S_1, S_2, \ldots, S_k$
foreach $\theta \in \Theta$ do
    for $i = 1..k$ do
        $h_{i,\theta} = \mathcal{A}(S \setminus S_i; \theta)$
        $error(\theta) = \frac{1}{k} \sum_{i=1}^{k} \mathcal{L}_{S_i}(h_{i,\theta})$
Output:
  $\theta^* = \underset{\theta}{\operatorname{argmin}}[error(\theta)]$
  $h_{\theta^*} = \mathcal{A}(S; \theta^*)$
```

Cross-validation performance

- Estimating the prediction error

$$
\begin{aligned}
CV(f) &= \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(y^i, f_{k(i)}(x^i)) \\
&= \frac{1}{k}\sum_{l=1}^{k}\mathbb{E}(f|D_l)
\end{aligned}
$$

  - where, $f_{k(i)}$ is the k_i-th part of the data removed
  - k_i is the fold in which i is
  - D_l is the fold l
- Estimating the expected prediction error

$$Error = \mathbb{E}[L(Y, f(X))]$$

Cross-validation issues

- The training set becomes $(k-1) * n/k$
  - small training set may lead to biased estimator of the error
- A special case of the k-fold cross-validation is the **leave-one-out (LDO)**; i.e., $k = n$
  - approximately unbiased of the expected prediction error
  - potential high variance, since the training sets are similar to each other
  - computation can be very difficult
- In practice, k is set up to 5 or 10.

Bootstrap

- Randomly draws datasets with replacement from the training set
- Repeats **B** times (often, $B = 100$), which leads to **B** models
- Leave-one-out bootstrap error
  - for each training point i, predicts with the $b_i < B$ models that did not have i in their training set
  - computes the average prediction errors
- This leads for training set that has $0.632 * n$ distinct examples. Why?

$$\begin{aligned}\mathbb{P}(i \in x_k) &= 1 - (1 - \tfrac{1}{n})^n \\ &\approx 1 - e^{-1} \\ &= 0.632\end{aligned}$$

- It has a high computational cost

Outline

1 Introduction

2 Supervised Linear Model

3 Use Case

4 Model Assessment

5 **References**

References

- Marianthi Markatou et al. “Analysis of Variance of Cross-Validation Estimators of the Generalization Error”. In: *Journal of Machine Learning Research* 6 (2005), pp. 1127–1168
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- Hal Daume III. *A Course in Machine Learning*. 2nd. Self-published, 2017. URL: http://ciml.info/dl/v0_99/ciml-v0_99-all.pdf

1. **Noise**: session 2.3
2. **Overfitting**: session 2.4
3. **Bias-variance trade-off**: session 5.9
4. **Holdout method**: session 2.5
5. **Cross-validation**: session 5.6
6. **Assessing model performance**: session 5.5

References

- Trevor Hastie, Robert Tibshirani, and Jerome Friedman. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. 2nd. Springer, 2016. URL: `https://web.stanford.edu/~hastie/Papers/ESLII.pdf`

1. **Overfitting**: session 7.1
2. **Bias-variance trade-off**: sessions 2.9, 7.2, and 7.3
3. **Cross-validation**: session 7.10
4. **Bootstrap**: session 7.11