4장 *Fundamentals of machine learning*

"지혜로운 자는 꿈을 확신하며 준비한다..."

This chapter covers

- Forms of machine learning beyond classification and regression
- Formal evaluation procedures for machine-learning models
- Preparing data for deep learning
- Feature engineering
- Tackling overfitting
- The universal workflow for approaching machine-learning problems

4.1 Four branches of machine learning

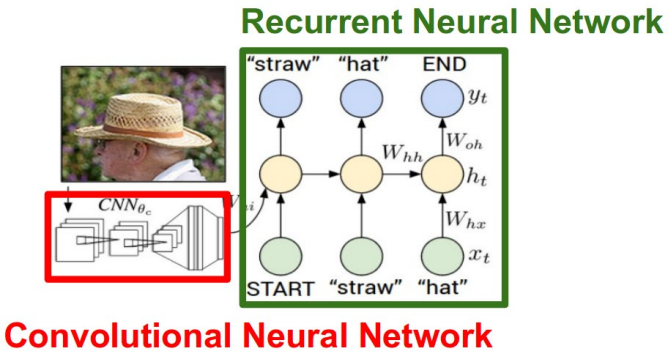
- examples: binary classification, multiclass classification, and scalar regression.
- All three are instances of *supervised learning*, where the goal is to learn the relationship between training inputs and training targets.
- Supervised learning is just the *tip of the iceberg*—machine learning is a vast field with a complex subfield taxonomy.
- Machine-learning algorithms generally fall into four broad categories: supervised learning, unsupervised learning, self-supervised learning, reinforcement learning

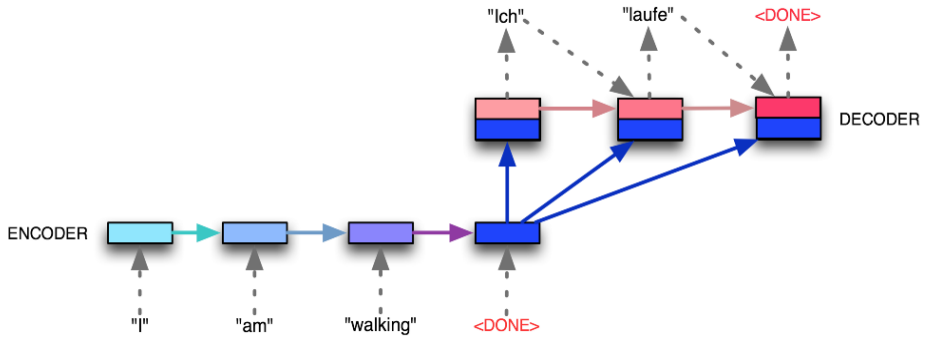
4.1 Four branches of machine learning

4.1.1 Supervised learning

- map input data to known targets (also called *annotations*), given a set of examples (often annotated by humans)
- optical character recognition, speech recognition, image classification, and language translation
- more exotic variants:
  - *Sequence generation* — predict a caption describing it, repeatedly predicting a word or token in a sequence

Describing images

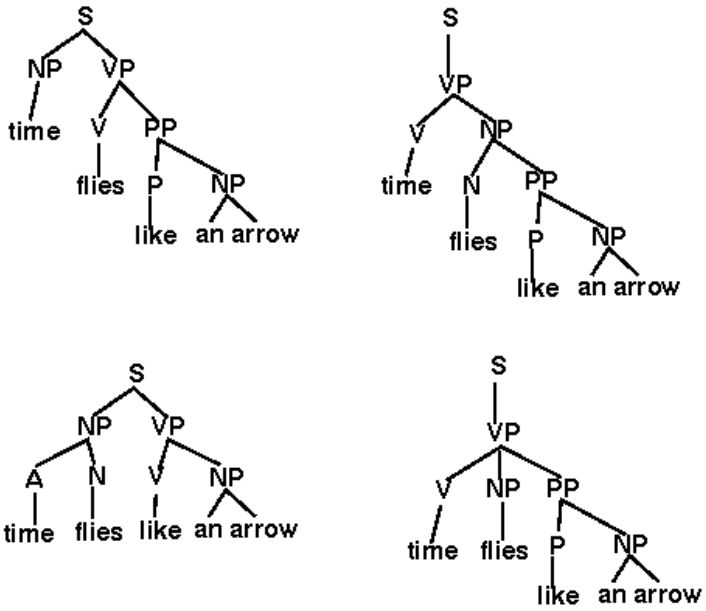


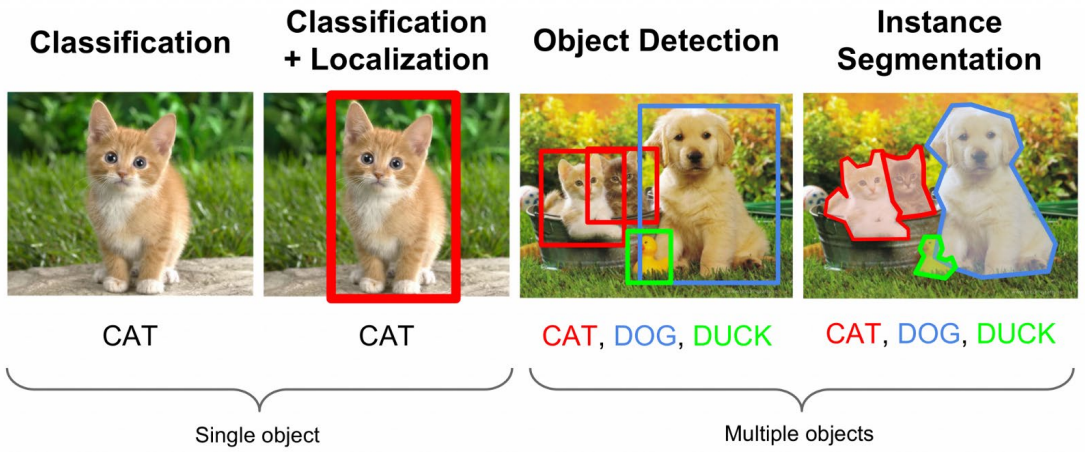


4.1 Four branches of machine learning

4.1.1 Supervised learning

- *Syntax tree prediction*—Given a sentence, predict its decomposition into a syntax tree.
- *Object detection*—Given a picture, draw a bounding box around certain objects inside the picture. This can also be expressed as a classification problem or as a joint classification and regression problem, where the bounding-box coordinates are predicted via vector regression.
- *Image segmentation*—Given a picture, draw a pixel-level mask on a specific object.

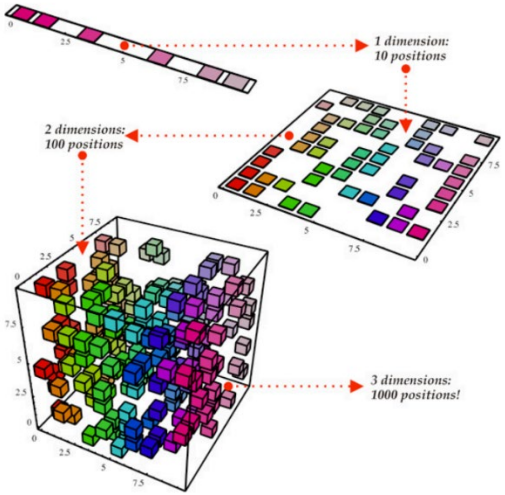


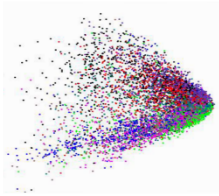


4.1 Four branches of machine learning

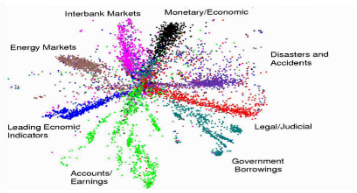
4.1.2 Unsupervised learning

- input data without the help of any targets
- data visualization, data compression, or data denoising, or to better understand the correlations
- better understanding a dataset before attempting to solve a supervised-learning problem.
- *Dimensionality reduction* and *clustering* are well-known categories of unsupervised learning.

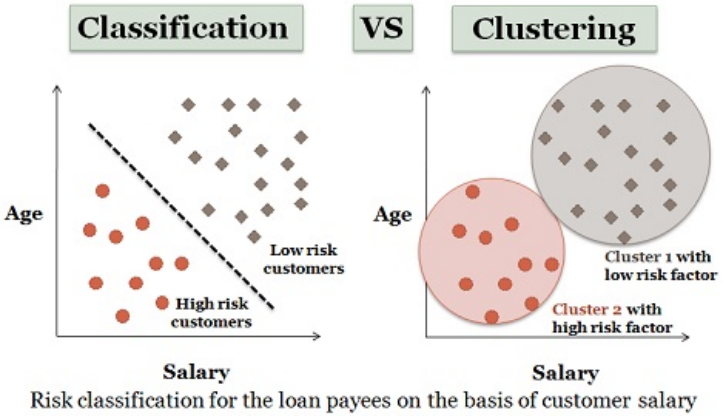




PCA



Auto Encoder

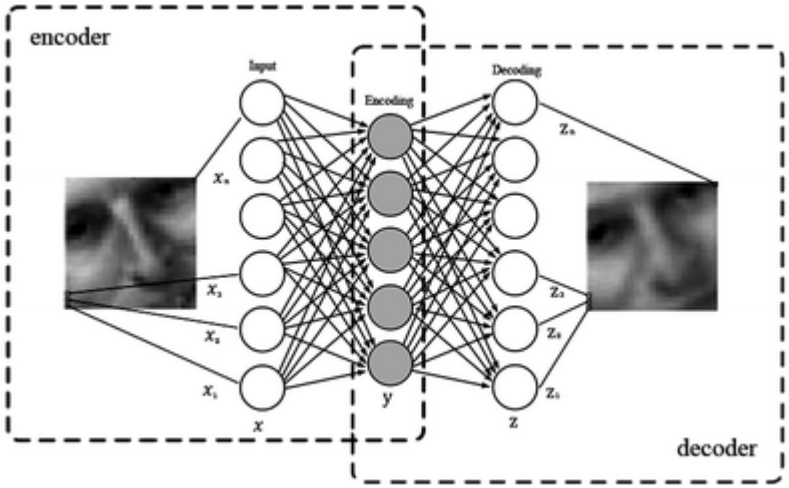


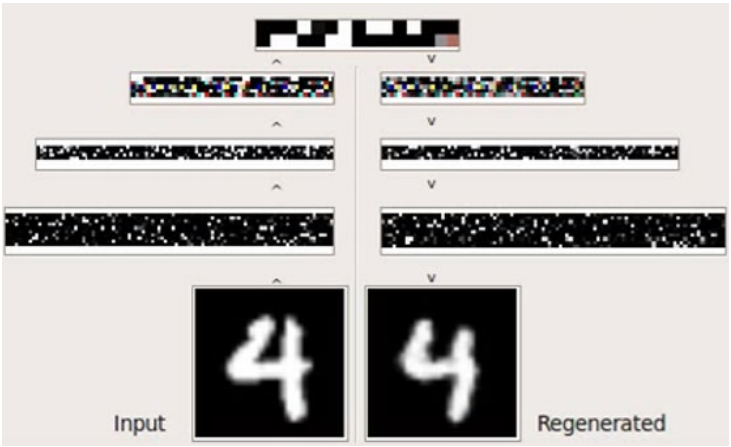
Risk classification for the loan payees on the basis of customer salary

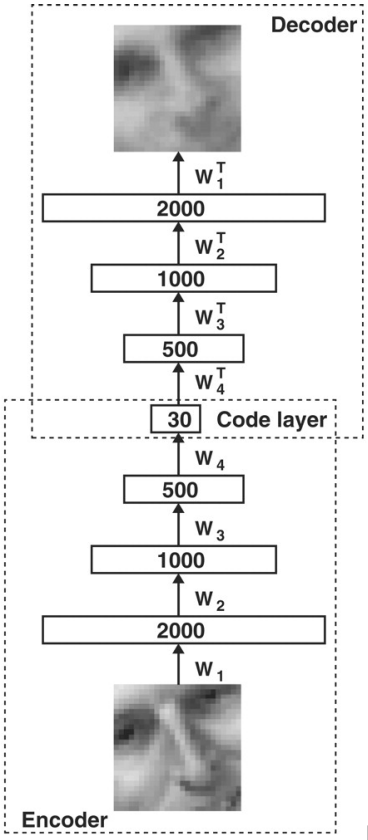
4.1 Four branches of machine learning

4.1.3 Self-supervised learning

- Self-supervised learning is supervised learning without human-annotated labels but still labels from the input data.
- *autoencoders* - the generated targets are the input
- predict the next frame in a video, given past frames, or the next word in a text, given previous words



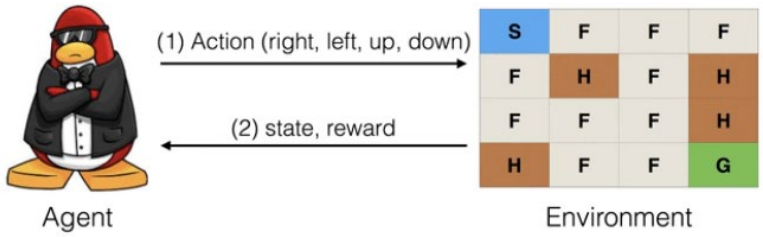




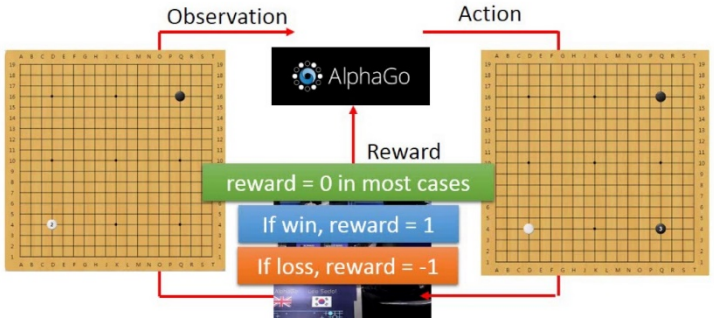
4.1 Four branches of machine learning

4.1.4 Reinforcement learning

- Google DeepMind successfully applied it to learning to play Atari games
- *agent* receives information about its environment and learns to choose actions that will maximize some reward.
- self-driving cars, robotics, resource management, education, and so on.



Learning to paly Go



4.1 Four branches of machine learning

Classification and regression glossary

- *Sample* or *input*—One data point that goes into your model.
- *Prediction* or *output*—What comes out of your model.
- *Target*—The truth. What your model should ideally have predicted, according to an external source of data.
- *Prediction error* or *loss value*—A measure of the distance between your model's prediction and the target.
- *Classes*—A set of possible labels to choose from in a classification problem. ("dog" and "cat" classes)
- *Label*—A specific instance of a class annotation in a classification problem.
- *Ground-truth* or *annotations*—All targets for a dataset, typically collected by humans.
- *Binary classification*—each input sample should be categorized into two exclusive categories.
- *Multiclass classification*—each input sample should be categorized into more than two categories
- *Multilabel classification*—each input sample can be assigned multiple labels. For instance, a given image may contain both a cat and a dog and should be annotated both with the "cat" label and the "dog" label.
- *Scalar regression*—A task where the target is a continuous scalar value, Predicting house
- *Vector regression*—A task where the target is a set of continuous values (the coordinates of a bounding box in an image)
- *Mini-batch* or *batch*—A small set of samples (typically between 8 and 128) that are processed simultaneously by the model. The number of samples is often a power of 2, to facilitate memory allocation on GPU. When training, a mini-batch is used to compute a single gradient-descent update applied to the weights of the model.

4.2 Evaluating machine-learning models

- split the data into a training set, a validation set, and a test set
- after just a few epochs, all three models began to *overfit*
- the goal is *generalize*—perform well on never-before-seen
- The following sections look at strategies for mitigating overfitting and maximizing generalization.
- how to measure generalization: how to evaluate machine-learning models.

4.2 Evaluating machine-learning models

4.2.1 Training, validation, and test sets

- Evaluating a model: splitting the available data into training, validation, and test
- developing a model - tuning its configuration: for example, choosing the number of layers or the size of the layers (called the *hyper-parameters* of the model, to distinguish them from the *parameters*, which are the network's weights), form of *learning*: a search
- never-before-seen dataset to evaluate the model: the test dataset, *no* information about the test set

4.2 Evaluating machine-learning models

4.2.1 Training, validation, and test sets

- three classic evaluation recipes: simple hold-out validation, K-fold validation, and iterated K-fold validation with shuffling.

SIMPLE HOLD-OUT VALIDATION

- Set apart some fraction of your data as your test set.
- Train on the remaining data, and evaluate on the test set.

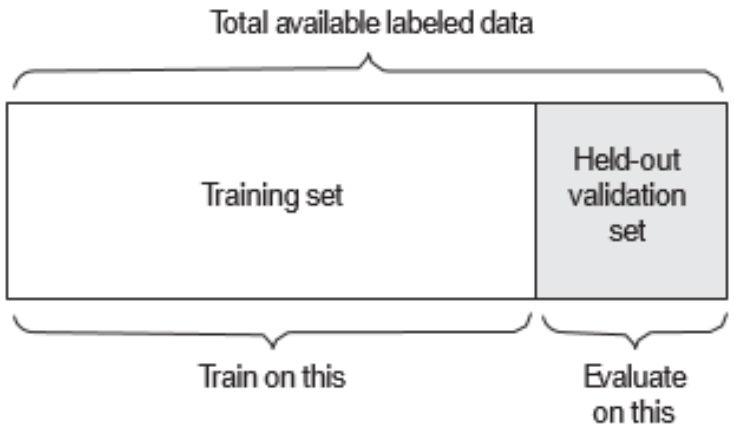


Figure 4.1 Simple hold-out validation split

4.2 Evaluating machine-learning models

4.2.1 Training, validation, and test sets

In [36]:
```
english_grade = [100,90,92,95,70,84,80,75,89]
E = np.array(english_grade)
print(E)

np.random.shuffle(E)
print(E)
```

```
[100  90  92  95  70  84  80  75  89]
[ 75 100  90  92  84  95  89  80  70]
```

Listing 4.1 Hold-out validation

```
num_validation_samples = 10000
np.random.shuffle(data)
validation_data = data[:num_validation_samples] # 검증
data = data[num_validation_samples:]  # 훈련
training_data = data[:] # 훈련
model = get_model() # 미리 정의된 model 호출
model.train(training_data)
validation_score = model.evaluate(validation_data)
# At this point you can tune your model,
# retrain it, evaluate it, tune it again...

model = get_model() # 최종 테스트
model.train(np.concatenate([training_data, validation_data])) # 훈련 + 검증
test_score = model.evaluate(test_data) # 새로운 test data
```

4.2 Evaluating machine-learning models

4.2.1 Training, validation, and test sets

K-FOLD VALIDATION

- split your data into K partitions of equal size.
- for each partition `i`, train a model on the remaining $K - 1$ partitions, and evaluate it on partition `i`.
- Schematically, K-fold cross-validation looks like figure 4.2.

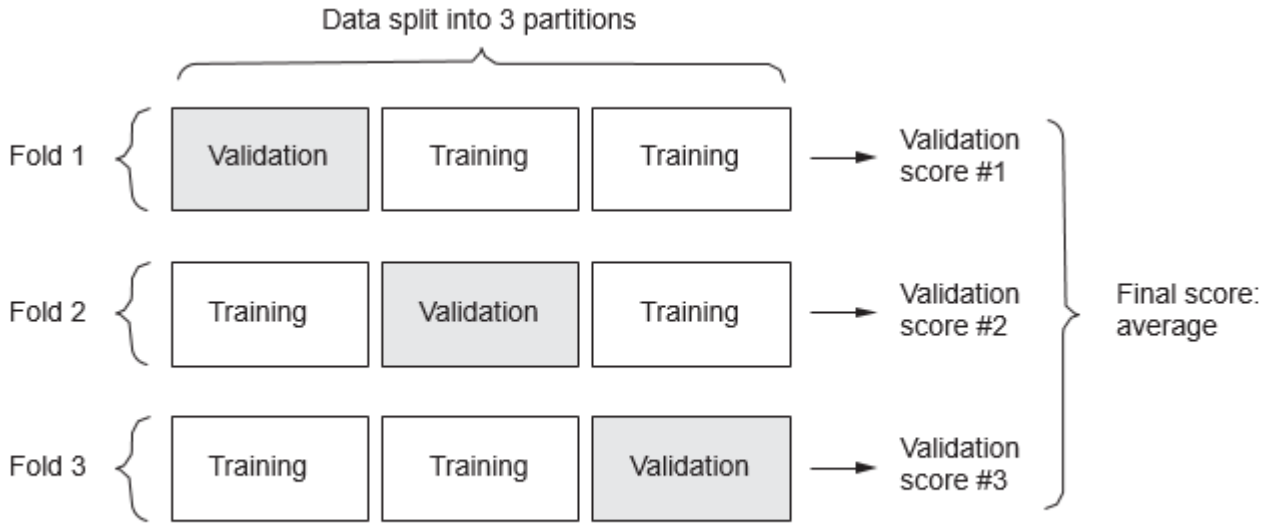


Figure 4.2 Three-fold validation

4.2 Evaluating machine-learning models

4.2.1 Training, validation, and test sets

- **Listing 4.2 K-fold cross-validation**

```
import numpy as np
k = 4
num_val_samples = len(train_data)
np.random.shuffle(data)
validation_scores = []
for fold in range(k):
    validation_data = data[num_validation_samples * fold:num_validation_samples * (fold+1)]
    training_data=data[:num_validation_samples*fold]+data[num_validation_samples*(fold + 1):]
    model = get_model()
    model.train(training_data)
    validation_score = model.evaluate(validation_data)
    validation_scores.append(validation_score)

validation_score = np.average(validation_scores)
model = get_model()
model.train(data)
test_score = model.evaluate(test_data)
```

ITERATED K-FOLD VALIDATION WITH SHUFFLING

- $P \times K$ models (where P is the number of iterations you use)

4.2 Evaluating machine-learning models

4.2.2 Things to keep in mind

Keep an eye out for the following when you're choosing an evaluation protocol:

- *Data representativeness* — 80% of training set containing only classes 0–7, whereas 20% of test set contains only classes 8–9 (ridiculous mistake), *randomly shuffle* your data before splitting it into training and test sets.
- *The arrow of time* — predict the future given the past (for example, **tomorrow's weather**, **stock movements**, and so on), *not* randomly shuffle your data before splitting it, test set is *posterior* to the data in the training set.
- *Redundancy in your data* — Make sure your training set and validation set are disjoint (not redundancy between the training and validation sets).

4.3 Data preprocessing, feature engineering, and feature learning

- How do you prepare the input data and targets before feeding them into a neural network?
- Many data-preprocessing and feature-engineering techniques are domain specific (for example, specific to text data set or image data set).

4.3.1 Data preprocessing for neural networks

- Data preprocessing: vectorization, normalization, handling missing values, feature selection, and feature extraction.

VECTORIZATION

- *data vectorization* - All inputs and targets in a neural network must be tensors of floating-point data (or, in specific cases, tensors of integers) for weights and a lot of functions. - sound, images, text
- one-hot encoding - tensor of `float32` data

4.3 Data preprocessing, feature engineering, and feature learning

VALUE NORMALIZATION

- digit-classification - 0–255 grayscale values → `float32` values in the 0–1 range
- predicting house prices - variety of ranges → normalize each feature independently with a standard deviation of 1 and a mean of 0
  - *Take small values*—Typically, most values should be in the 0–1 range.
  - *Be homogenous*— all features should take values in roughly the same scale
- normalization practice:
  - Normalize each feature independently to have a mean of 0.
  - Normalize each feature independently to have a standard deviation of 1.

This is easy to do with Numpy arrays:

```
x -= x.mean(axis=0)
x /= x.std(axis=0)
```

4.3 Data preprocessing, feature engineering, and feature learning

HANDLING MISSING VALUES

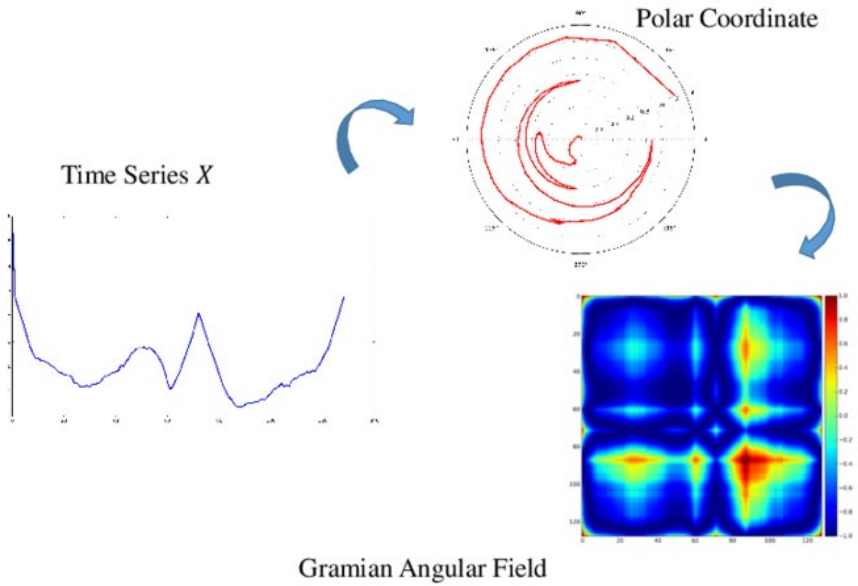
- missing values - input missing values as 0, with the condition that 0 isn't already a meaningful value, ignoring the value.
- missing values in the test data, but no missing values in the train data - copy some missing data samples to the train data
- Define ignoring the value - ?, #, !, -9

(abnegation, expunge, grandiloquent) 약탈, 말소, 과장

4.3 Data preprocessing, feature engineering, and feature learning

4.3.2 Feature engineering

- *Feature engineering* - the process of transformations of input data for better result before it goes into the model
- Make model's job easier
- image of a clock and can output the time of day (see figure 4.3).
- raw pixels < (x, y) coordinates < angle `theta` of each clock hand.
- making a problem easier by expressing it in a simpler way



Raw data: pixel grid		
Better features: clock hands' coordinates	{x1: 0.7, y1: 0.7} {x2: 0.5, y2: 0.0}	{x1: 0.0, y2: 1.0} {x2: -0.38, 2: 0.32}
Even better features: angles of clock hands	theta1: 45 theta2: 0	theta1: 90 theta2: 140

Figure 4.3 Feature engineering for reading the time on a clock

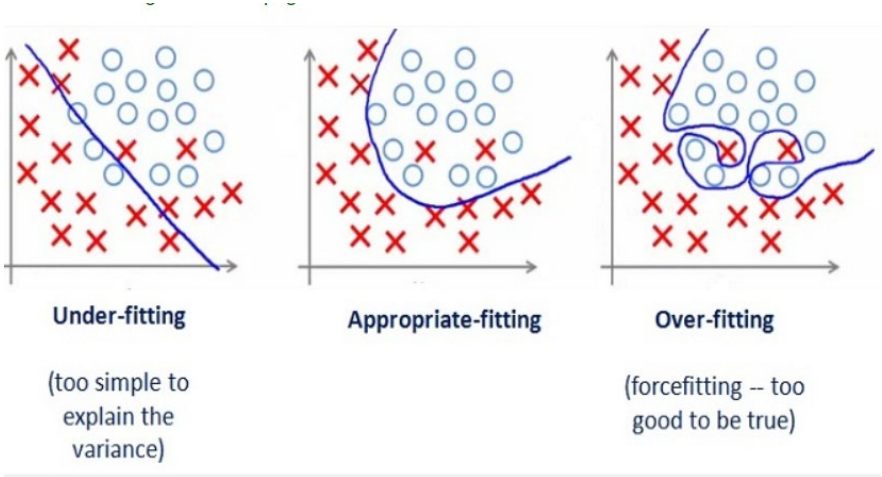
4.3 Data preprocessing, feature engineering, and feature learning

4.3.2 Feature engineering

- Before deep learning, feature engineering used to be critical
- MNIST digit-classification problem - number of loops in a digit image, the height of each digit in an image, a histogram of pixel values, and so on.
- Deep learning ***removes*** the need for most feature engineering by automatic extraction of useful features from raw data.
- Does this mean you don't have to worry about feature engineering as long as you're using deep neural networks? No, for two reasons:
  - Good features still allow you to solve problems more elegantly while using fewer resources (clock example).
  - Good features let you solve a problem with far less data.

4.4 Overfitting and underfitting

- In all three examples—predicting movie reviews, topic classification, and house-price regression—the model quickly started to overfit to the training data.
- Optimization refers to the process of adjusting a model to get the best performance possible on the training data.
- Generalization refers to how well the trained model performs on test data.
- underfit: the network hasn't yet modeled all relevant patterns in the training data.
- A model trained on more data will naturally generalize better.
- The processing of fighting overfitting this way is called regularization.



4.4 Overfitting and underfitting

4.4.1 Feature engineering Reducing the network's size

- reduce the size of the model: number of layers and the number of units per layer
- model's large *memorization capacity*: perfect dictionary-like mapping between training samples and their targets
- but the real challenge is generalization, not fitting.
- no magical formula to determine the right number of layers or the right size for each layer.
- start with relatively few layers and parameters, and increase the size of the layers

4.4 Overfitting and underfitting

4.4.1 Feature engineering Reducing the network's size

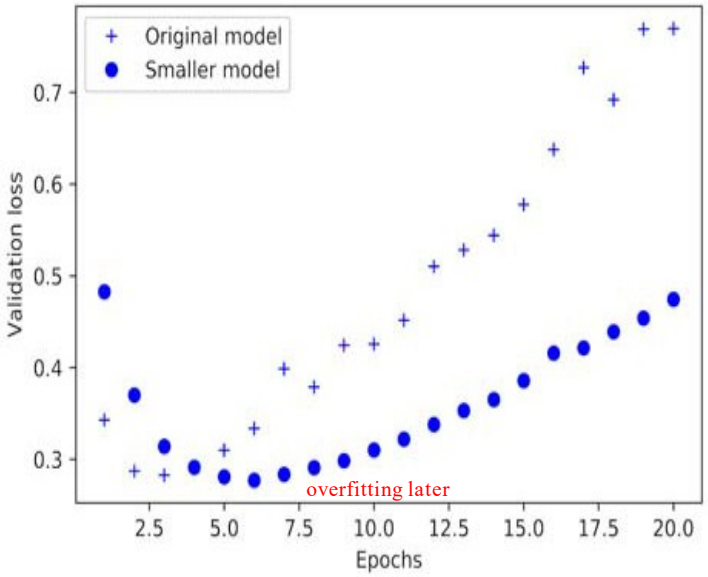


Figure 4.4 Effect of model capacity on validation loss: trying a smaller model

Listing 4.3 Original model

```
from keras import models
from keras import layers
model = models.Sequential()
model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))
```

Listing 4.4 Version of the model with lower capacity

```
model = models.Sequential()
model.add(layers.Dense(4, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(4, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))
```

4.4 Overfitting and underfitting

4.4.1 Feature engineering Reducing the network's size

Listing 4.5 Version of the model with higher capacity

```
model = models.Sequential()
model.add(layers.Dense(512, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(512, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))
```

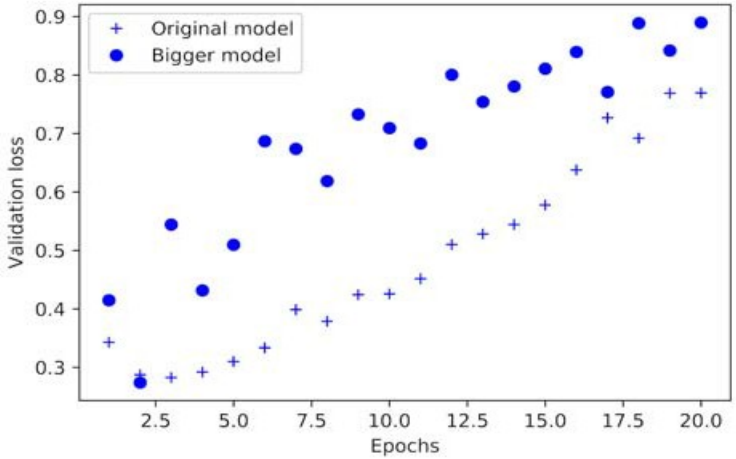


Figure 4.5 Effect of model capacity on validation loss: trying a bigger model

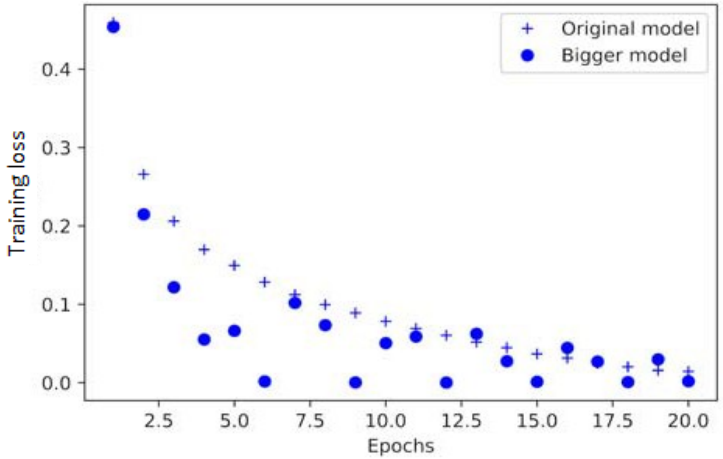


Figure 4.6 Effect of model capacity on training loss: trying a bigger model

4.4 Overfitting and underfitting

4.4.2 Adding weight regularization

- *Occam's razor* : given two explanations for something, the explanation most likely to be correct is the simplest one, 노트르담 대성당 화재 원인(사고 vs. 테러), 영화선택
- neural networks: Simpler models are less likely to overfit than complex ones.
- A *simple model* - fewer parameters
- *weight regularization* - adding to the loss function of the network a *cost* associated with having large weights:
  - *L1 regularization* —The cost added is proportional to the *absolute value of the weight coefficients* (the *L1 norm* of the weights) .
  - *L2 regularization* (*weight decay*)—The cost added is proportional to the *square of the value of the weight coefficients* (the *L2 norm* of the weights).

4.4 Overfitting and underfitting

- L1 regularization (λ) with Back-Propagation

current values of the weights are (6.0, -2.0, 4.0), λ=0.1

add 0.1 * [|6.0| + | -2.0| + |4.0|] = 0.1 * (6.0 + 2.0 + 4.0) = 0.1 * 12.0 = 1.20 to E

(0.1 *[|4.0| + | -4.0| + |4.0|]=1.2의 경우와 동일)

$$E = \frac{1}{2} * \sum (t_k - o_k)^2 + \lambda * \sum |w_i|$$

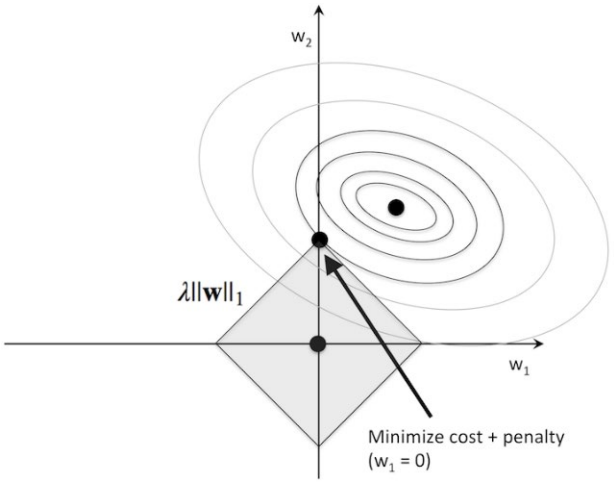
squared error — L1 weight penalty

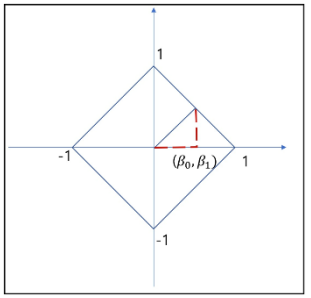
$$\Delta w_{jk} = -1 * \eta * \left[x_j * (o_k - t_k) * o_k * (1 - o_k) \right] \pm \lambda \Big]$$

$\frac{\partial E}{\partial w_{jk}}$ gradient

learning rate — signal

$$w_{jk} = w_{jk} + \Delta w_{jk}$$





L1: $||\beta||_1 = |\beta_0| + |\beta_1| = 1$

4.4 Overfitting and underfitting

- L2 regularization (λ) with Back-Propagation

current values of the weights are (5.0, -3.0, 2.0), λ=0.1

add 0.1*[(5.0)^2 + (-2.0)^2 + (2.0)^2]=0.1 * (25.0 + 4.0 + 4.0) = 0.1 * 33.0 = 3.30 to *E*

(0.1 *[(3.0)^2 + (-3.0)^2 + (3.0)^2]=2.7과 차이)

$$E = \frac{1}{2} * \sum (t_k - o_k)^2 + \frac{\lambda}{2} * \sum w_i^2$$

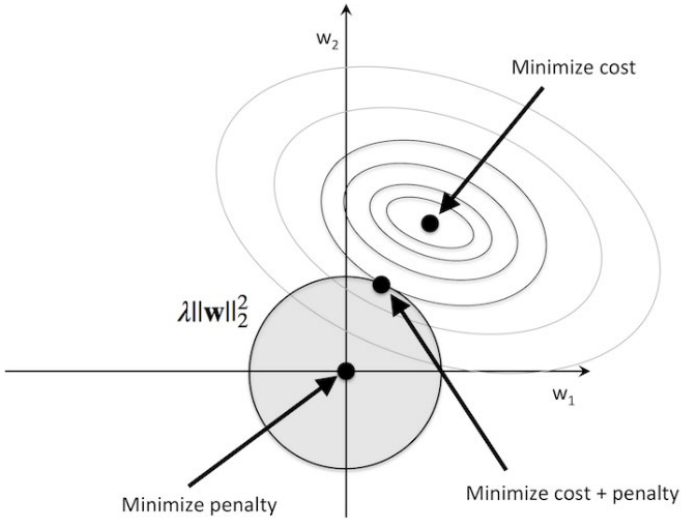
plain error　　weight penalty

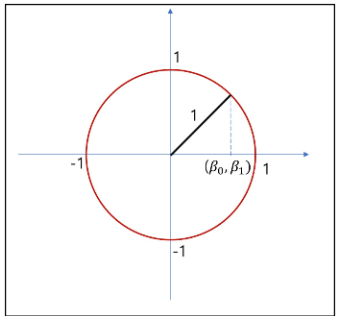
elegant math　　simple math

$$\frac{\partial E}{\partial w_{jk}}$$ gradient

$$\Delta w_{jk} = -\eta * [x_j * (o_k - t_k) * o_k * (1 - o_k)] + [\lambda * w_{jk}]$$

learning rate　　signal





L2: $||\beta||_2 = \sqrt{(\beta_0)^2 + (\beta_1)^2} = 1$

4.4 Overfitting and underfitting

- L1은 특정 weight를 0으로 바꿀 수 있기 때문에 sparse한 형태(**feature selection**)가 될 수 있다.

> *a = (0.25, 0.25, 0.25, 0.25)*
>
> *b = (-0.5, 0.5, 0.0, 0.0)*

이 두 벡터의 $L1$ norm을 구하면,

$$||a||_1 = |0.25| + |0.25| + |0.25| + |0.25| = 1$$

$$||b||_1 = |-0.5| + |0.5| + |0.0| + |0.0| = 1$$

과 같이 같은 1이라는 숫자가 나오지만,

$L2$ norm을 구하면,

$$||a||_2 = \sqrt{0.25^2 + 0.25^2 + 0.25^2 + 0.25^2} = 0.5$$

$$||b||_2 = \sqrt{(-0.5)^2 + (0.5)^2 + 0^2 + 0^2} = 0.707$$

과 같이 다른 수가 나온다.

L1

SPARSITY: $(1, 0, 0, 1, 0)$

GOOD FOR FEATURE SELECTION

L2

SPARSITY: $(0.5, 0.3, -0.2, 0.4, 0.1)$

NORMALLY BETTER FOR TRAINING MODELS

$(1, 0) \rightarrow (0.5, 0.5)$

$1^2 + 0^2 = 1 \quad 0.5^2 + 0.5^2 = 0.5$

4.4 Overfitting and underfitting

- Weight regularization is added by passing *weight regularizer instances* to layers as keyword arguments. Let's add L2 weight regularization to the movie-review classification network.

Listing 4.6 Adding L2 weight regularization to the model

```
from keras import regularizers
model = models.Sequential()
model.add(layers.Dense(16,
          kernel_regularizer=regularizers.l2(0.001),
          activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16,
          kernel_regularizer=regularizers.l2(0.001),
          activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))
```

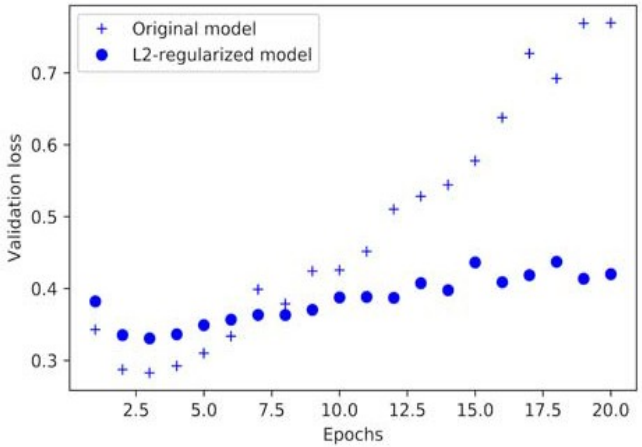


Figure 4.7 Effect of L2 weight regularization on validation loss

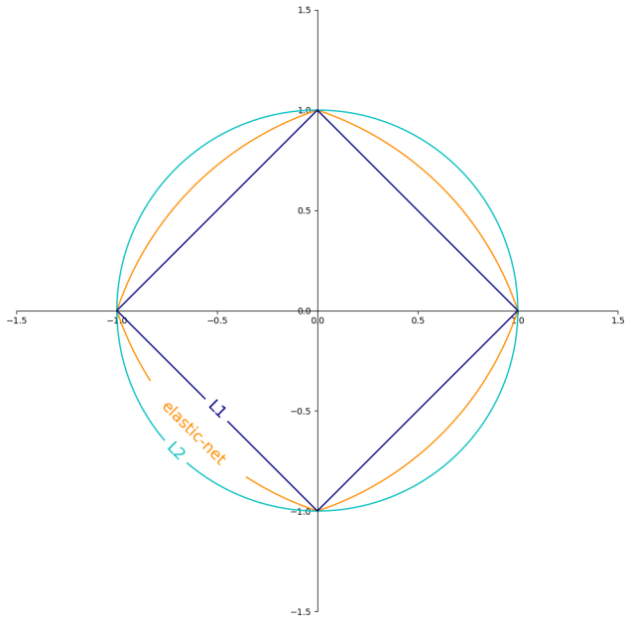
- `l2(0.001)` means every coefficient in the weight matrix of the layer will add `0.001 * weight_coefficient_value` to the total loss of the network
- Figure 4.7 shows the impact of the **L2** regularization penalty - more resistant to overfitting

4.4 Overfitting and underfitting

- As an alternative to L2 regularization, you can use one of the following Keras weight regularizers.

Listing 4.7 Different weight regularizers available in Keras

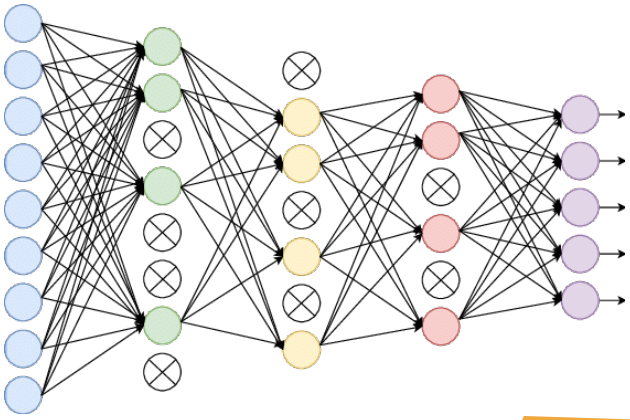
```
from keras import regularizers

regularizers.l1(0.001)

regularizers.l1_l2(l1=0.001, l2=0.001) #Elastic-net
```



4.4 Overfitting and underfitting

4.4.3 Adding dropout

- *Dropout* is one of the most effective and most commonly used regularization techniques for neural networks.
- Dropout, applied to a layer, consists of randomly *dropping out* (setting to zero) a number of output features of the layer during training.
- a given layer [0.2, 0.5, 1.3, 0.8, 1.1] → [0, 0.5, 1.3, 0, 1.1]
- The *dropout rate* is set between 0.2 and 0.5.



4.4 Overfitting and underfitting

4.4.3 Adding dropout

- In Keras, you can introduce dropout in a network via the `Dropout` layer, which is applied to the output of the layer right before it:

Listing 4.8 Adding dropout to the IMDB

```
model = models.Sequential()
model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dropout(0.5)) # 바로 전 출력층에 적용
model.add(layers.Dense(16, activation='relu'))
model.add(layers.Dropout(0.5)) # 바로 전 출력층에 적용
model.add(layers.Dense(1, activation='sigmoid'))
```

Figure 4.9 shows a plot of the results. Again, this is a clear improvement over the reference network

- these are the most common ways to prevent overfitting in neural networks:
  - Get more training data.
  - Reduce the capacity of the network.
  - Add weight regularization.
  - Add dropout.

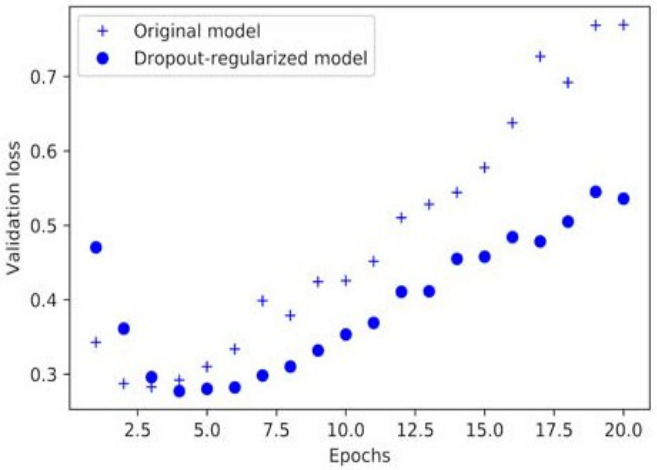


Figure 4.9 Effect of dropout on validation loss

4.5 The universal workflow of machine learning

- blueprint : problem definition, evaluation, feature engineering, and fighting overfitting.

4.5.1 Defining the problem and assembling a dataset

- First, you must define the problem at hand:
  - available training data - limiting factor (unless you have the means to pay people to collect data for you).
  - binary classification? Multiclass classification? Scalar regression? Vector regression? Multiclass, multilabel classification? Something else, like clustering, generation, or reinforcement learning? - Identifying the problem type
- hypotheses you make at this stage:
  - outputs can be predicted given your inputs.
  - available data is sufficiently informative to learn the relationship between inputs and outputs.

Table 4.1 Choosing the right last-layer activation and loss function for your model

Problem type	Last-layer activation	Loss function
Binary classification	`sigmoid`	`binary_crossentropy`
Multiclass, single-label classification	`softmax`	`categorical_crossentropy`
Multiclass, multilabel classification	`sigmoid`	`binary_crossentropy`
Regression to arbitrary values	None	`mse`
Regression to values between 0 and 1	`sigmoid`	`mse` or `binary_crossentropy`