Neural Network

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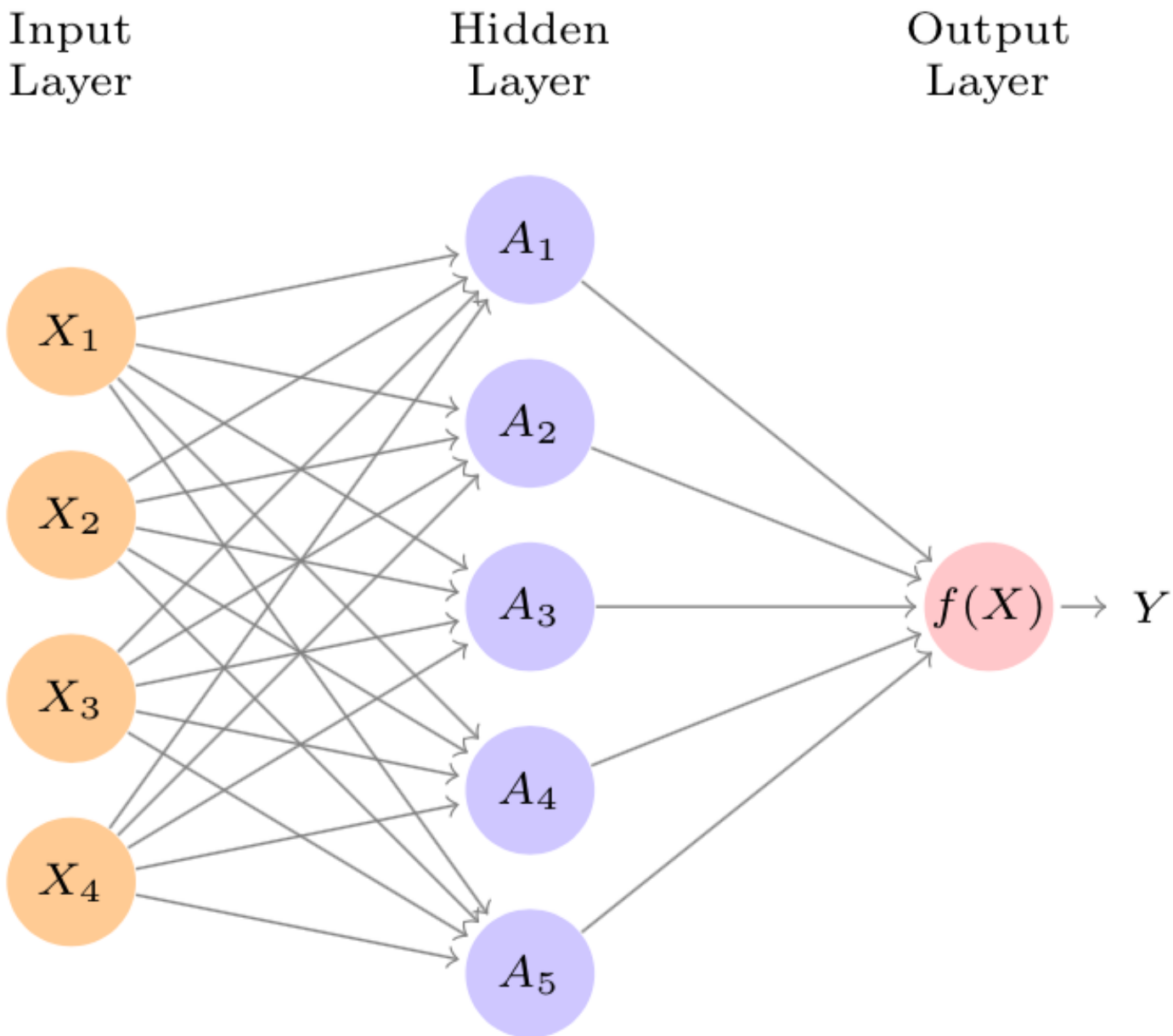
Contents of this week

- Basic Neural Network
- Convolutional Neural Network (CNN) and Recurrent Neural Network (RNN)
- Double Descent Phenomenon and Interpretation

Basic Neural Network

Single Layer Neural Network



Framework of Feed-Forward Neural Network

- A neural network takes an input vector of p variables $X = (X_1, X_2, \ldots, X_p)$ and builds a nonlinear function $f(X)$ to predict the response Y.
- The model is

$$f(X) = \beta_0 + \sum_{k=1}^{K} \beta_k h_k(X) = \beta_0 + \sum_{k=1}^{K} \beta_k g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_j\right). \quad (1)$$

- Hidden Layer: K activations $A_k, k = 1, 2, \ldots, K$ are

$$A_k = h_k(X) = g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_j\right). \quad (2)$$

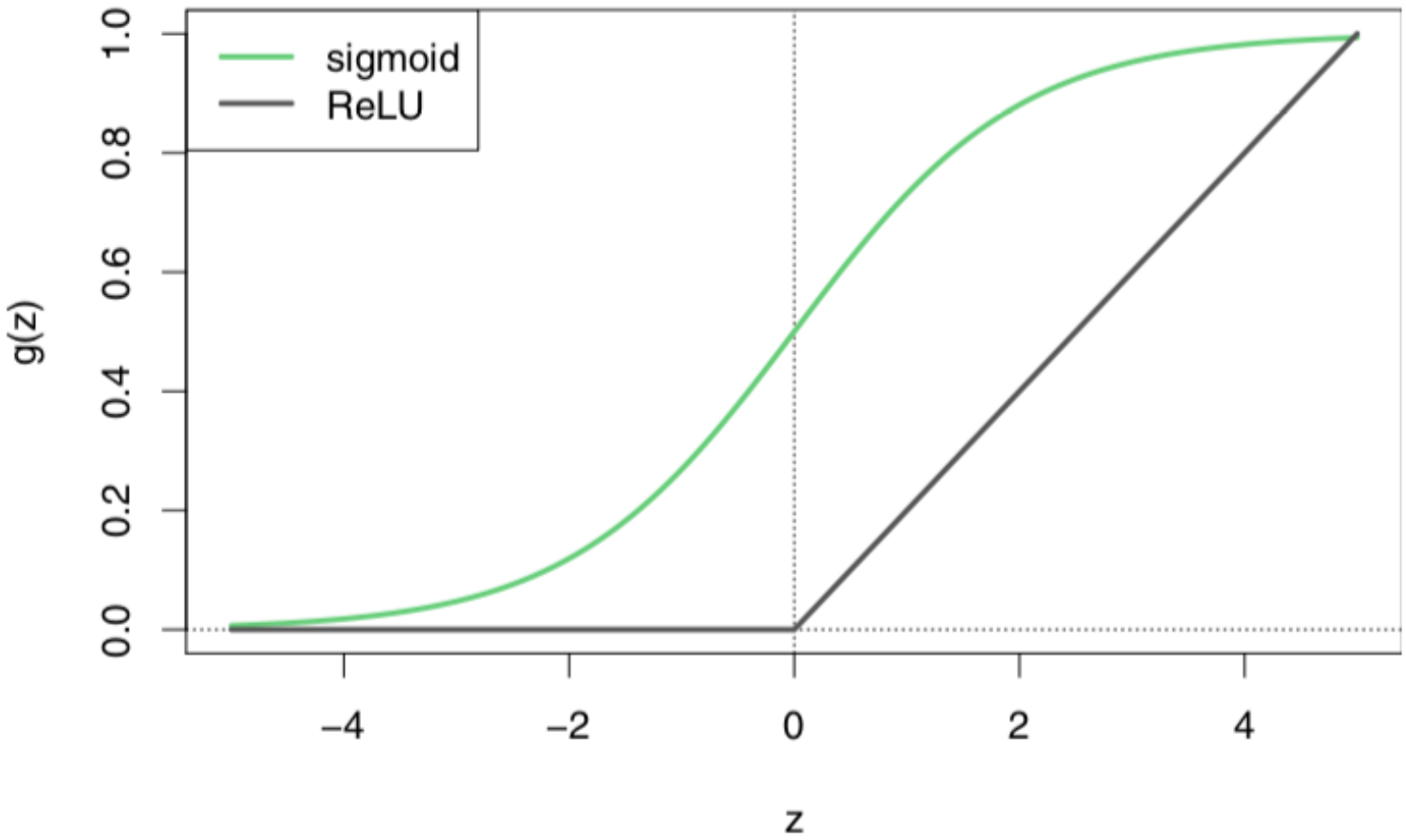
- The output layer:

$$f(X) = \beta_0 + \sum_{k=1}^{K} \beta_k A_k. \quad (3)$$

- In terms of minimizing a loss function, NN recovers the unknown weights parameters. For instance,

$$\sum_{i=1}^{n} (y_i - f(x_i))^2. \quad (4)$$

Activation Functions



Activation Functions

- The sigmoid activation function is

$$g(z) = \frac{e^z}{1 + e^z} = \frac{1}{1 + e^{-z}}. \tag{5}$$

- The ReLU (rectified linear unit) activation function is

$$g(z) = \begin{cases} 0, & z < 0 \\ z, & z \geq 0 \end{cases} \tag{6}$$

Nonlinearity of NN

The nonlinearity of NN in the activation function $g(\cdot)$ is essential. Consider an example with $p = 2$ input variables $X = (X_1, X_2)$ and $K = 2$ hidden units $h_1(X)$ and $h_2(X)$ with $g(z) = z^2$.

$$\begin{array}{lll} \beta_0 = 0, & \beta_1 = \frac{1}{4}, & \beta_2 = -\frac{1}{4}, \\ w_{10} = 0, & w_{11} = 1, & w_{12} = 1, \\ w_{20} = 0, & w_{21} = 1, & w_{22} = -1. \end{array} \tag{10.6}$$

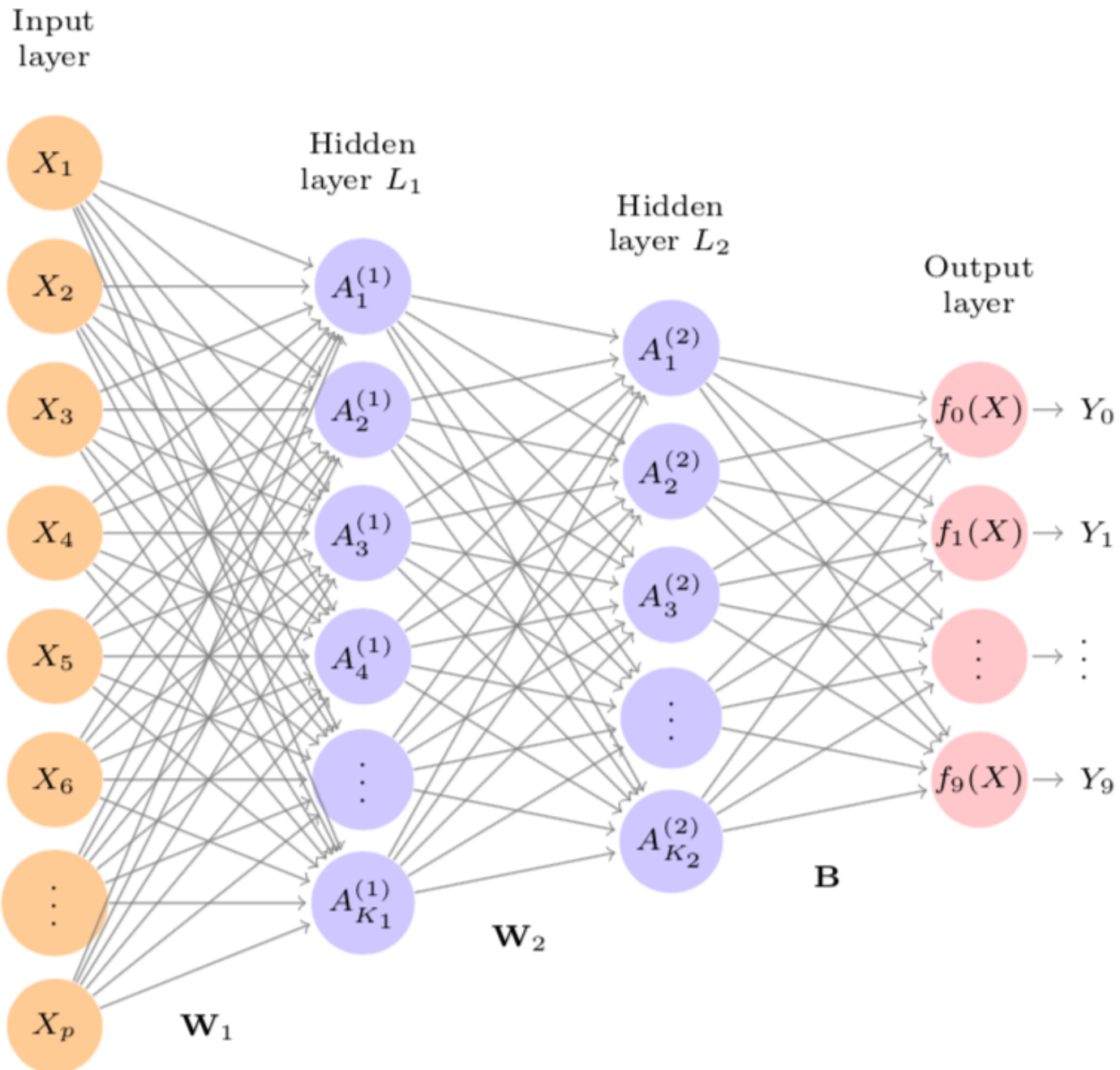
From (10.2), this means that

$$\begin{array}{rcl} h_1(X) & = & (0 + X_1 + X_2)^2, \\ h_2(X) & = & (0 + X_1 - X_2)^2. \end{array} \tag{10.7}$$

Then plugging (10.7) into (10.1), we get

$$\begin{array}{rcl} f(X) & = & 0 + \frac{1}{4} \cdot (0 + X_1 + X_2)^2 - \frac{1}{4} \cdot (0 + X_1 - X_2)^2 \\ & = & \frac{1}{4} \left[(X_1 + X_2)^2 - (X_1 - X_2)^2 \right] \\ & = & X_1 X_2. \end{array} \tag{10.8}$$

Multilayer Neural Network



Formulation of Multilayer NN

- It has two hidden layers L_1 (256 units) and L_2 (128 units) rather than one. Later we will see a network with seven hidden layers.
- It has ten output variables, rather than one. In this case the ten variables really represent a single qualitative variable and so are quite dependent. (We have indexed them by the digit class 0–9 rather than 1–10, for clarity.) More generally, in *multi-task learning* one can predict different responses simultaneously with a single network; they all have a say in the formation of the hidden layers.
- The loss function used for training the network is tailored for the multiclass classification task.

Formulation of Multilayer NN

The first hidden layer is as in (10.2), with

$$\begin{aligned} A_k^{(1)} &= h_k^{(1)}(X) \\ &= g(w_{k0}^{(1)} + \textstyle\sum_{j=1}^{p} w_{kj}^{(1)} X_j) \end{aligned} \tag{10.10}$$

for $k = 1, \ldots, K_1$. The second hidden layer treats the activations $A_k^{(1)}$ of the first hidden layer as inputs and computes new activations

$$\begin{aligned} A_\ell^{(2)} &= h_\ell^{(2)}(X) \\ &= g(w_{\ell 0}^{(2)} + \textstyle\sum_{k=1}^{K_1} w_{\ell k}^{(2)} A_k^{(1)}) \end{aligned} \tag{10.11}$$

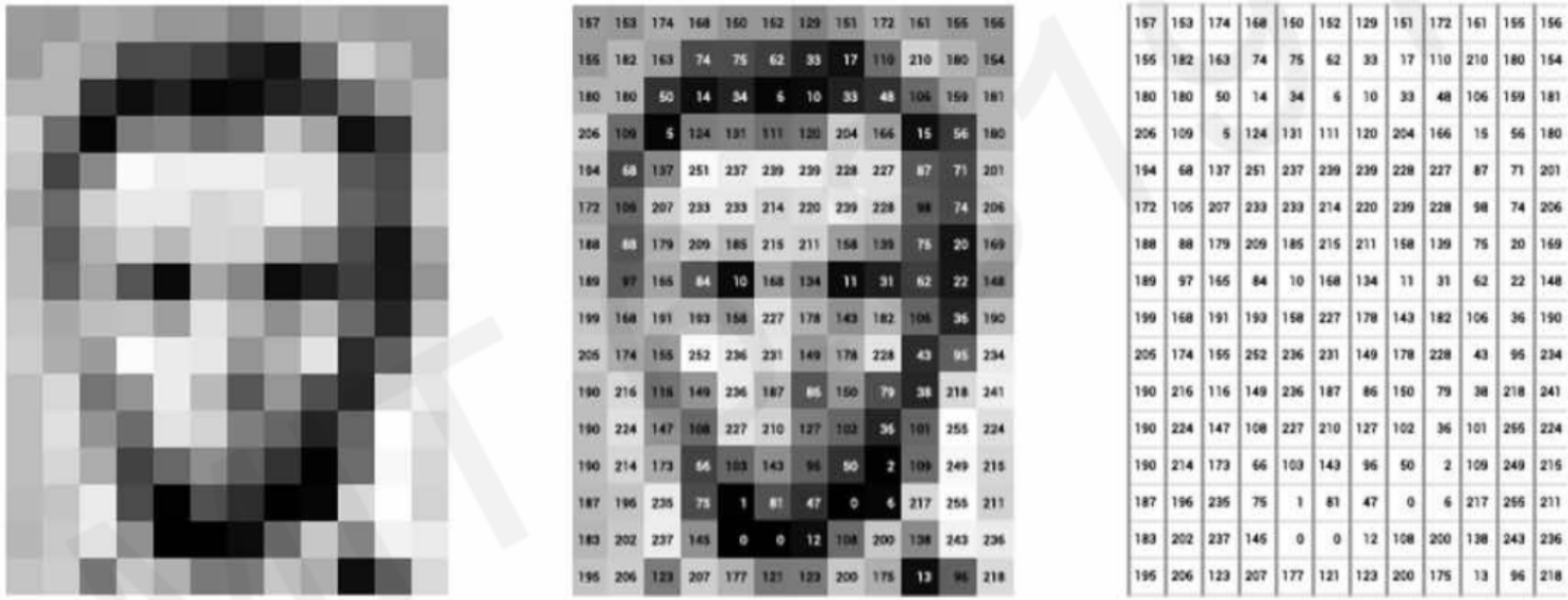
Convolutional Neural Network (CNN)

Aim and Content of CNN

Convolutional Neural Network is a structured neural network and aims to classify images. CNN consists of two parts:

- Feature Extraction: Convolutional Layers and Pooling Layers
- Fully Connected Neural Network with extracted features

Representation of Images in Computer



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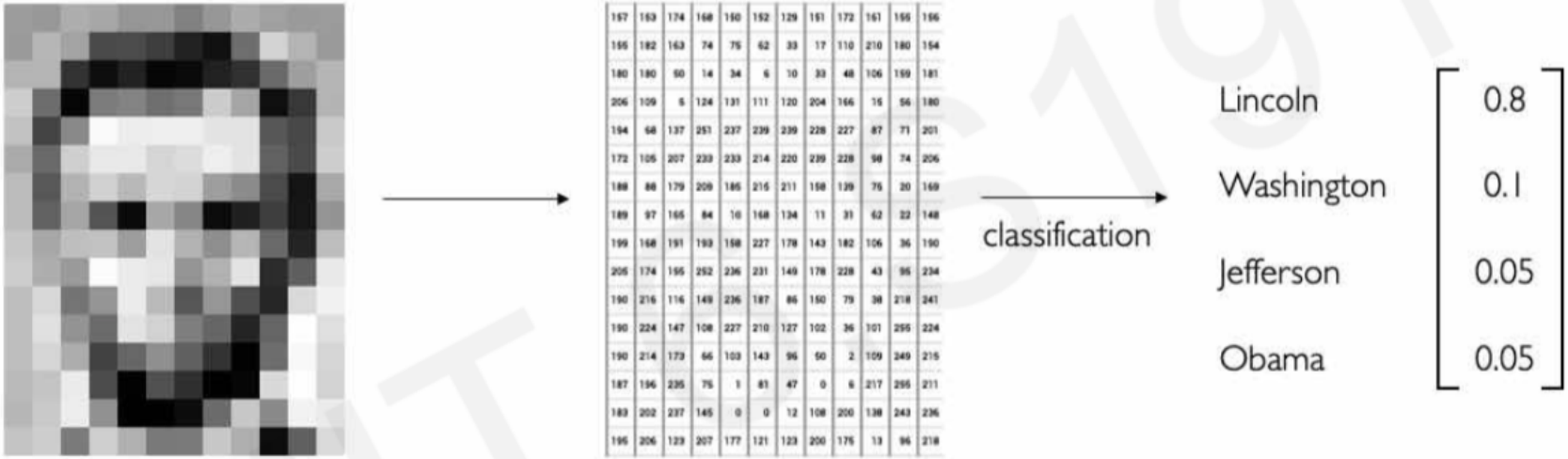
Computer Task for Images



- **Regression**: output variable takes continuous value
- **Classification**: output variable takes class label. Can produce probability of belonging to a particular class

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Feature Detection

The major challenge of image processing is feature detection.

Let's identify key features in each image category

Nose,
Eyes,
Mouth

Wheels,
License Plate,
Headlights

Door,
Windows,
Steps

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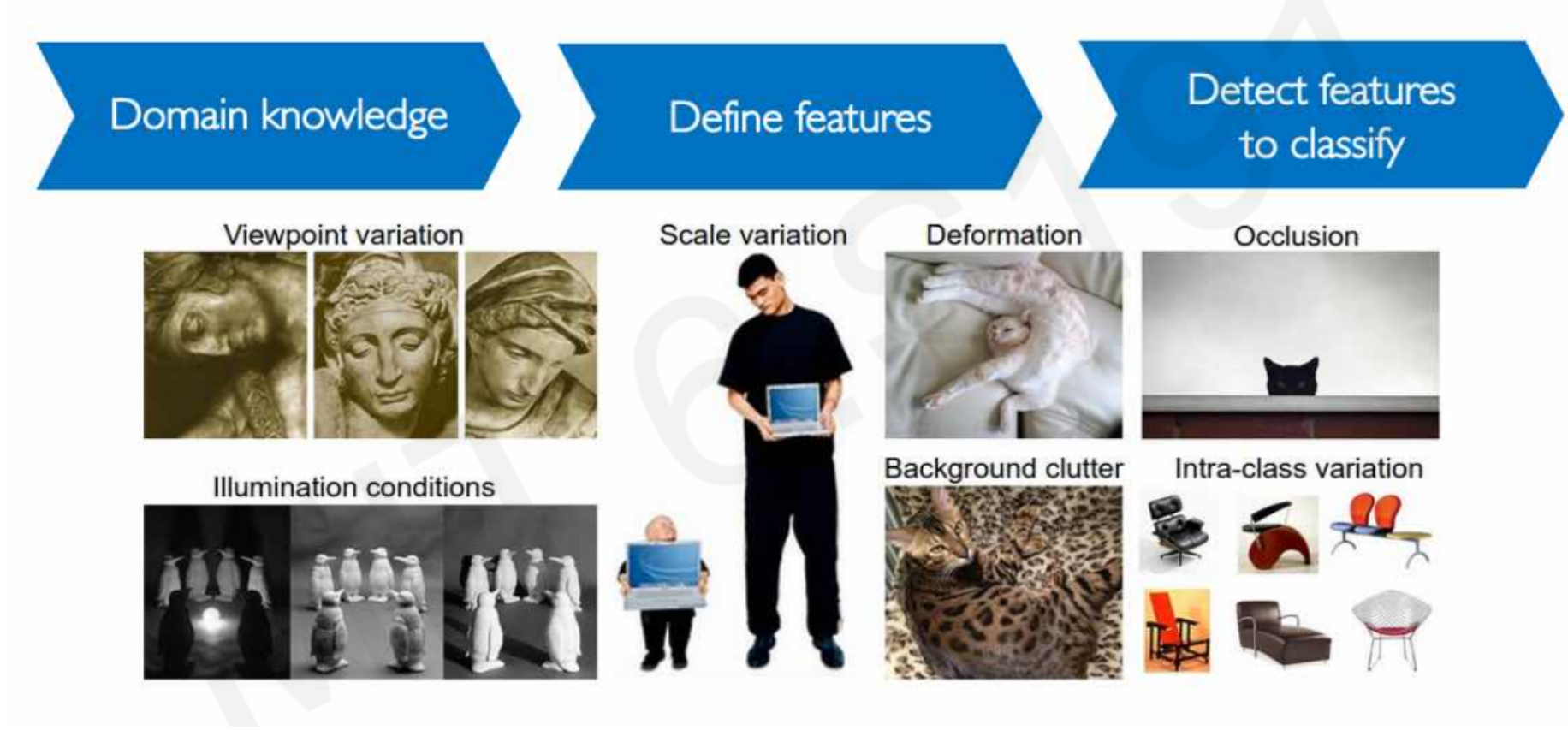
Manual Feature Extraction



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Manual Feature Extraction

The essential challenge of feature learning is to find features that are able to classify images.

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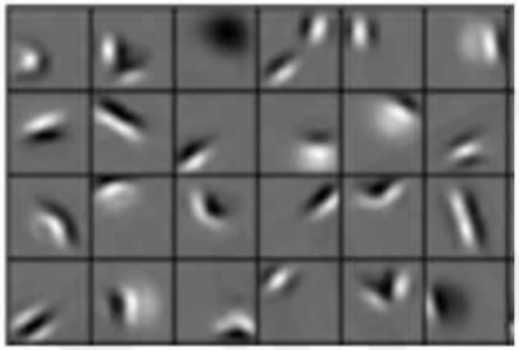
Feature Learning

Can we learn a **hierarchy of features** directly from the data instead of hand engineering?

Low level features



Edges, dark spots

Mid level features

Eyes, ears, nose

High level features

Facial structure

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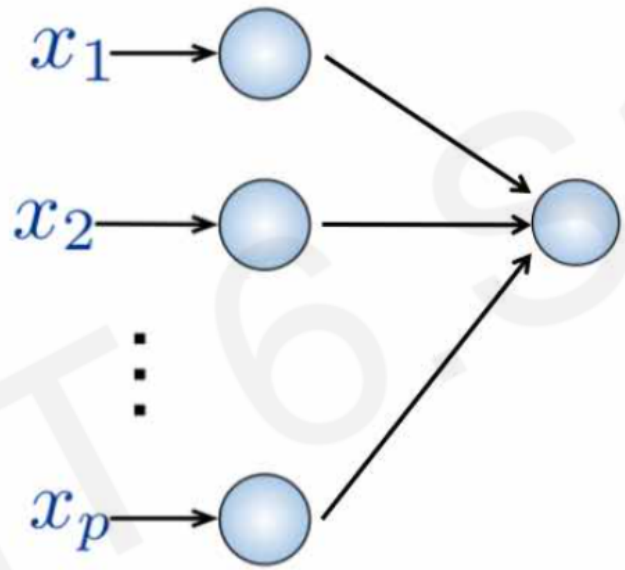
Failure of Fully Connected Neural Network

Input:

- 2D image
- Vector of pixel values



Fully Connected:

- Connect neuron in hidden layer to all neurons in input layer
- No spatial information!
- And many, many parameters!

How can we use **spatial structure** in the input to inform the architecture of the network?

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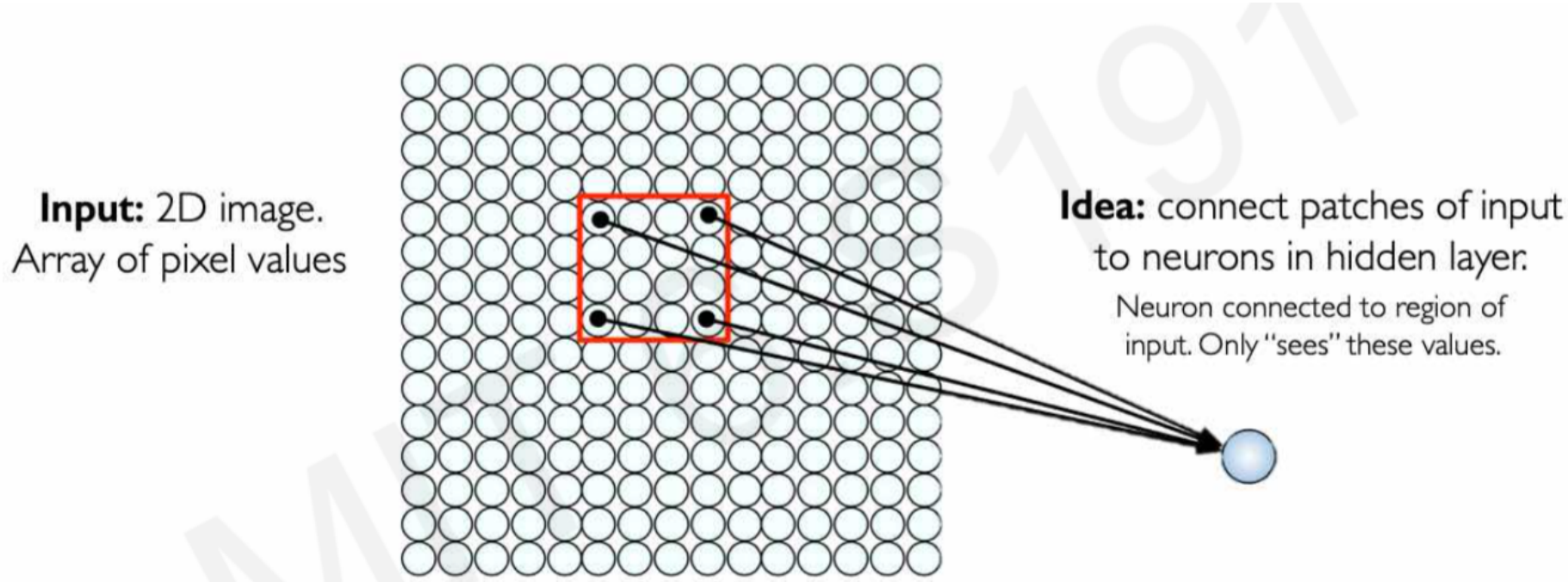
CNN: Imposing Spatial Structure



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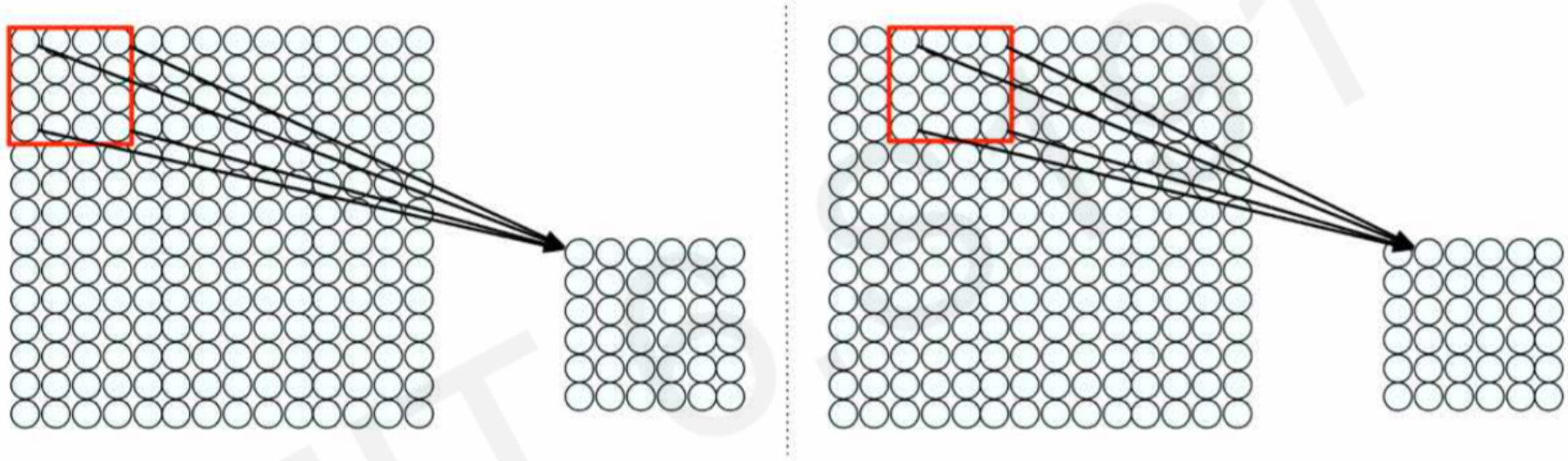
CNN: Imposing Spatial Structure



Connect patch in input layer to a single neuron in subsequent layer.
Use a sliding window to define connections.
How can we **weight** *the patch to detect particular features?*

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Feature Learning in CNN

1) Apply a set of weights – a filter – to extract **local features**

2) Use **multiple filters** to extract different features

3) Spatially **share** parameters of each filter
(features that matter in one part of the input should matter elsewhere)

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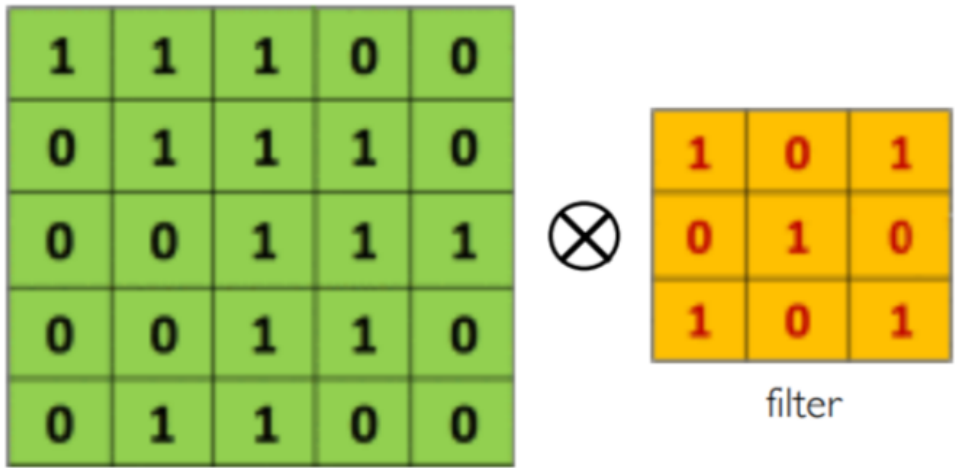
Illustration of Convolution Operation

Suppose we want to compute the convolution of a 5x5 image and a 3x3 filter:



We slide the 3x3 filter over the input image, element-wise multiply, and add the outputs...

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Illustration of Convolution Operation

We slide the 3x3 filter over the input image, element-wise multiply, and add the outputs:

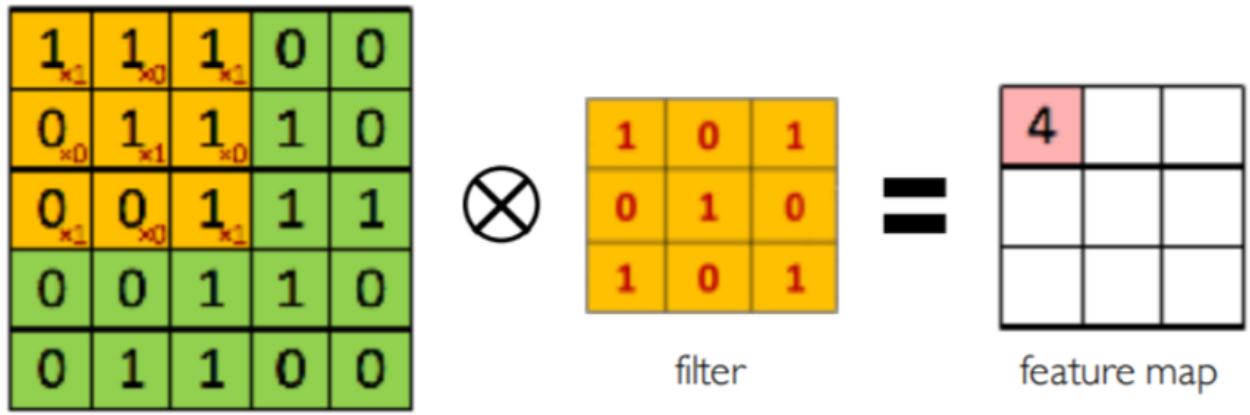

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Illustration of Convolution Operation

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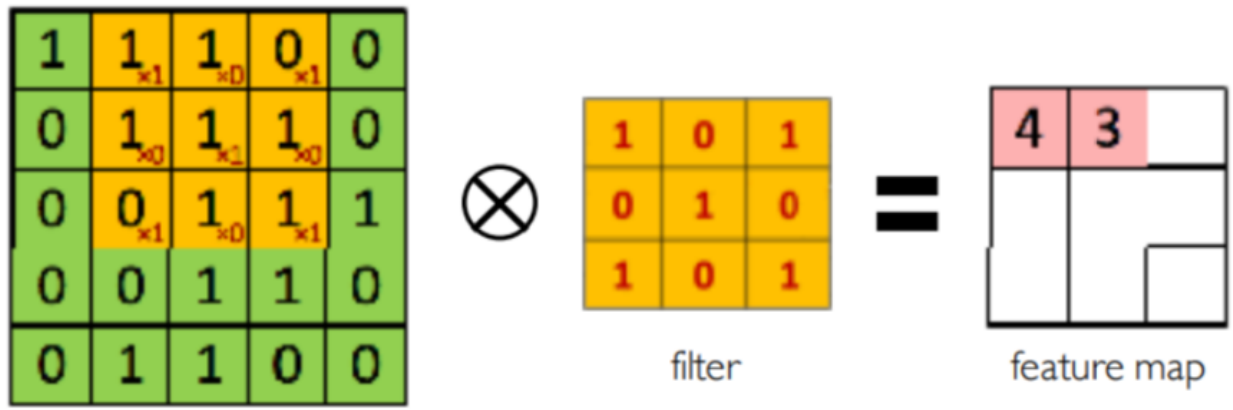

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Illustration of Convolution Operation

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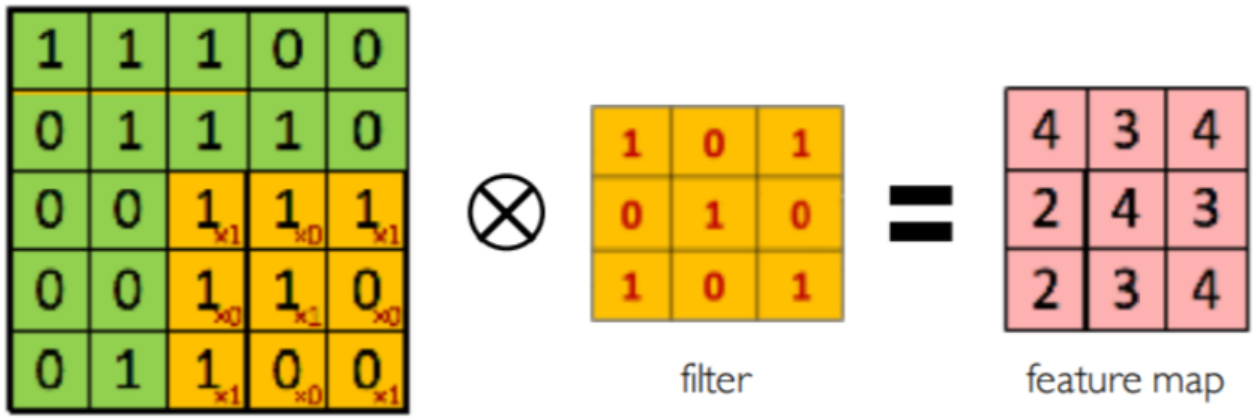

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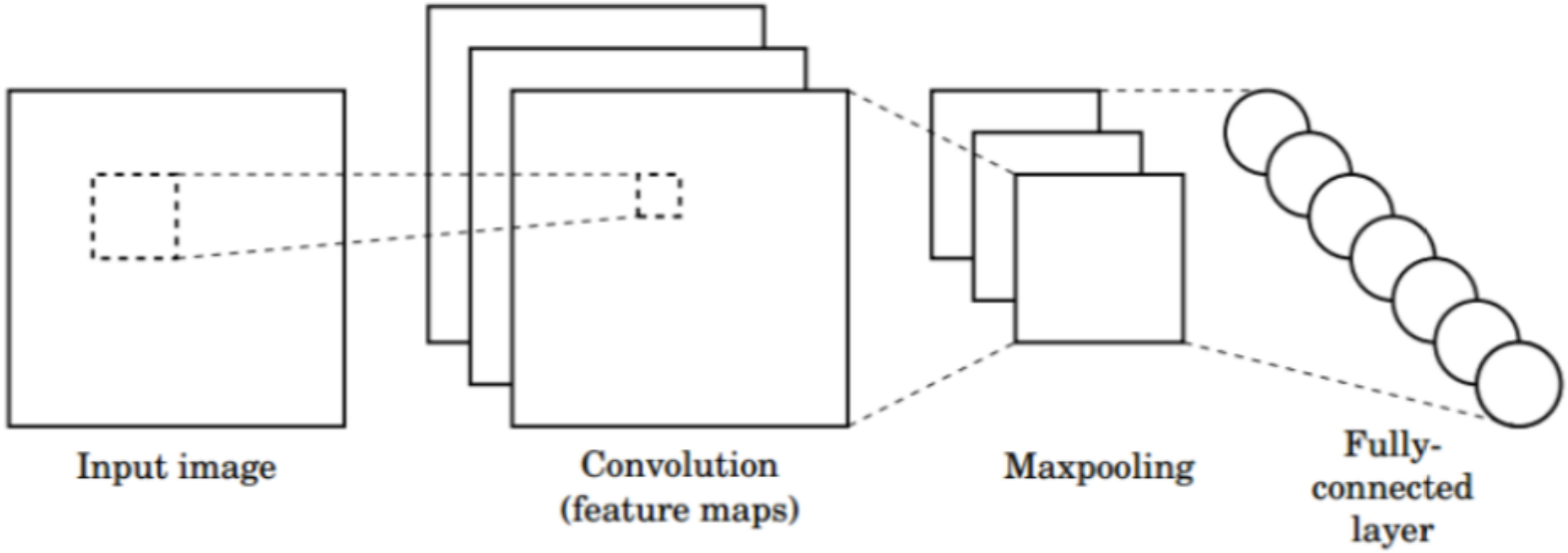
Summary of Feature Learning in CNN



1. **Convolution**: Apply filters with learned weights to generate feature maps.
2. **Non-linearity**: Often ReLU.
3. **Pooling**: Downsampling operation on each feature map.

Train model with image data.
Learn weights of filters in convolutional layers.

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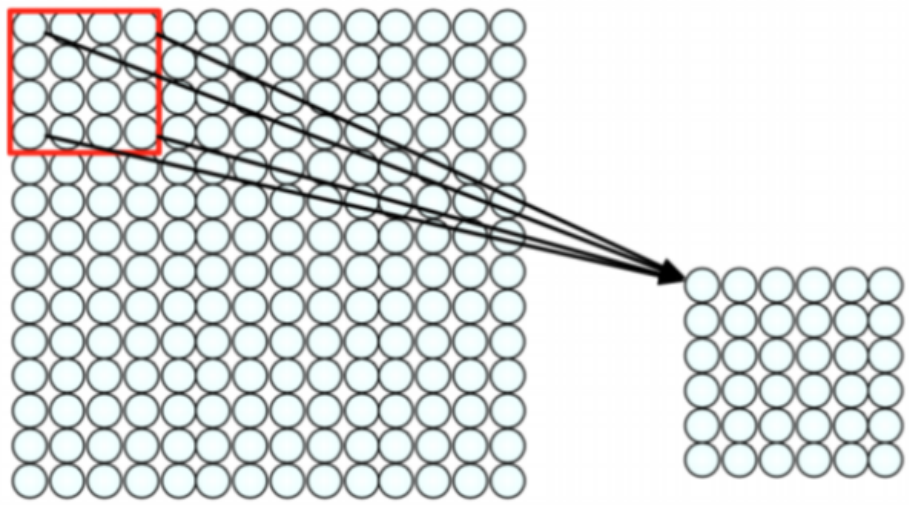
Formula of Convolution Operation



For a neuron in hidden layer:

- Take inputs from patch the neuron "sees"
- Compute weighted sum
- Apply bias

4x4 filter: matrix of weights θ_{ij}

$$\sum_{i=1}^{4}\sum_{j=1}^{4} \theta_{ij}\, x_{i+p,j+q} + b$$

for neuron (p,q) in hidden layer

applying a window of weights
computing linear combinations
activating with non-linear function

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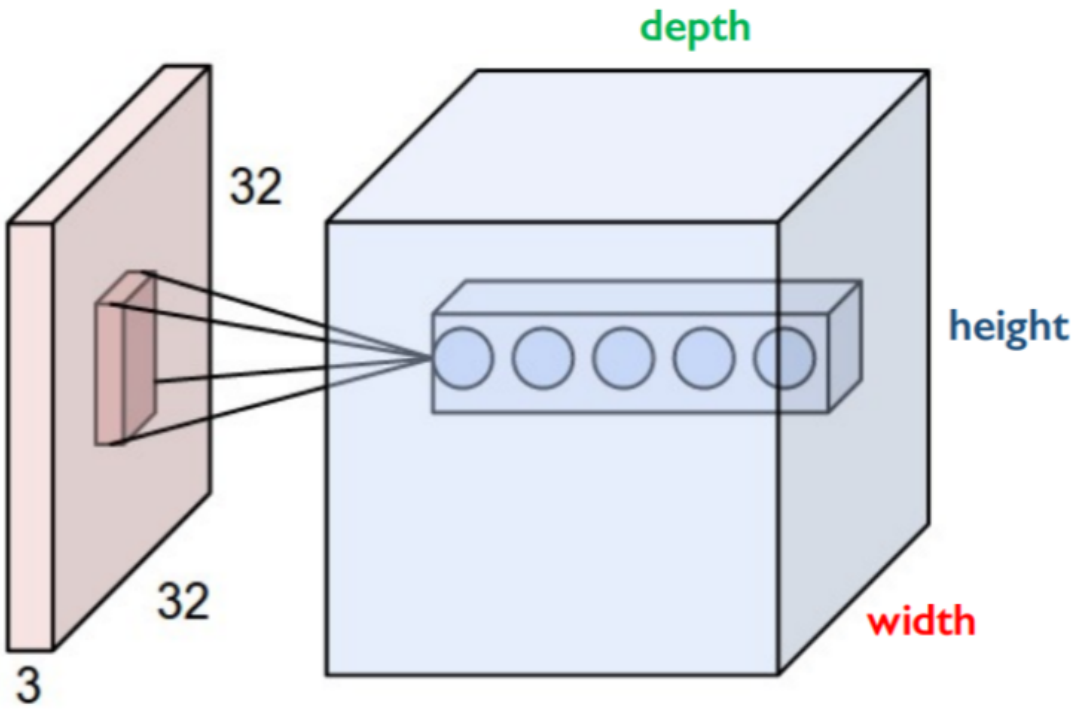
Spatial Positions of Neurons



Layer Dimensions:

$h \times w \times d$

where h and w are spatial dimensions
d (depth) = number of filters

Stride:

Filter step size

Receptive Field:

Locations in input image that a node is path connected to

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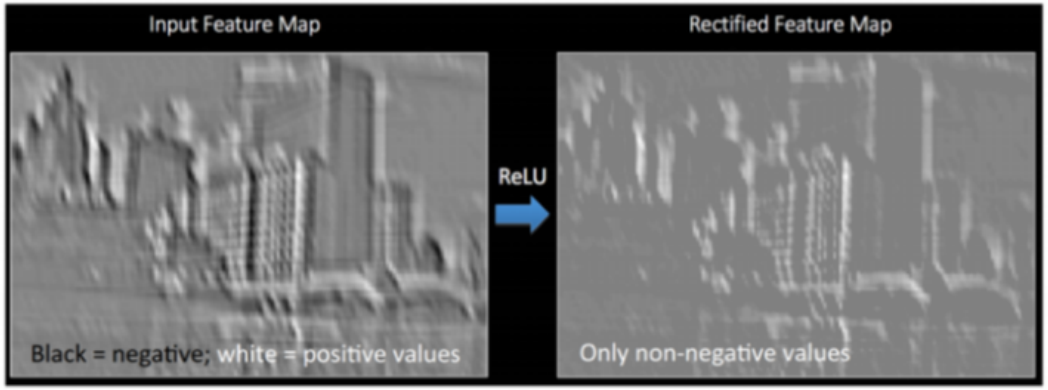
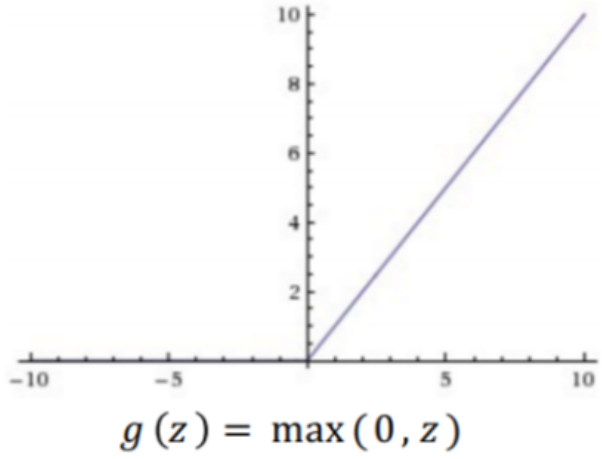
Nonlinearity via Activation Function

- Apply after every convolution operation (i.e., after convolutional layers)
- ReLU: pixel-by-pixel operation that replaces all negative values by zero. **Non-linear operation**



Rectified Linear Unit (ReLU)



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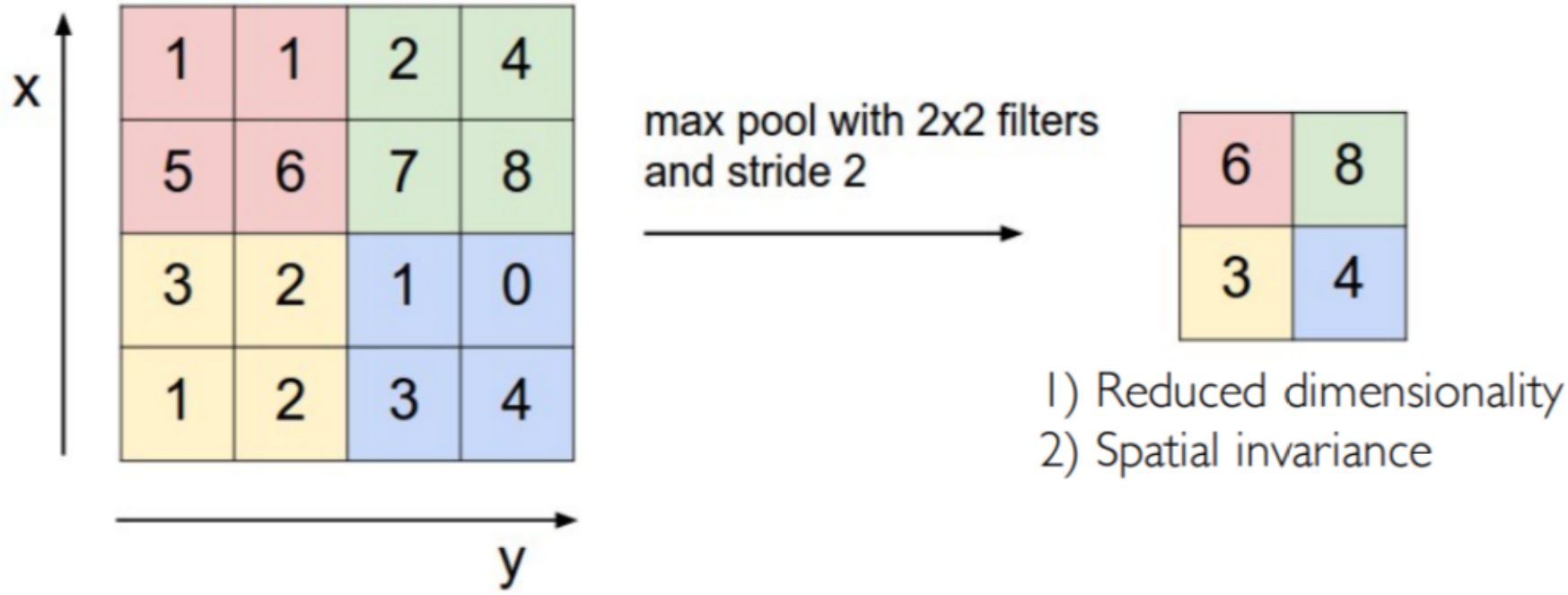
Max Pooling



How else can we downsample and preserve spatial invariance?

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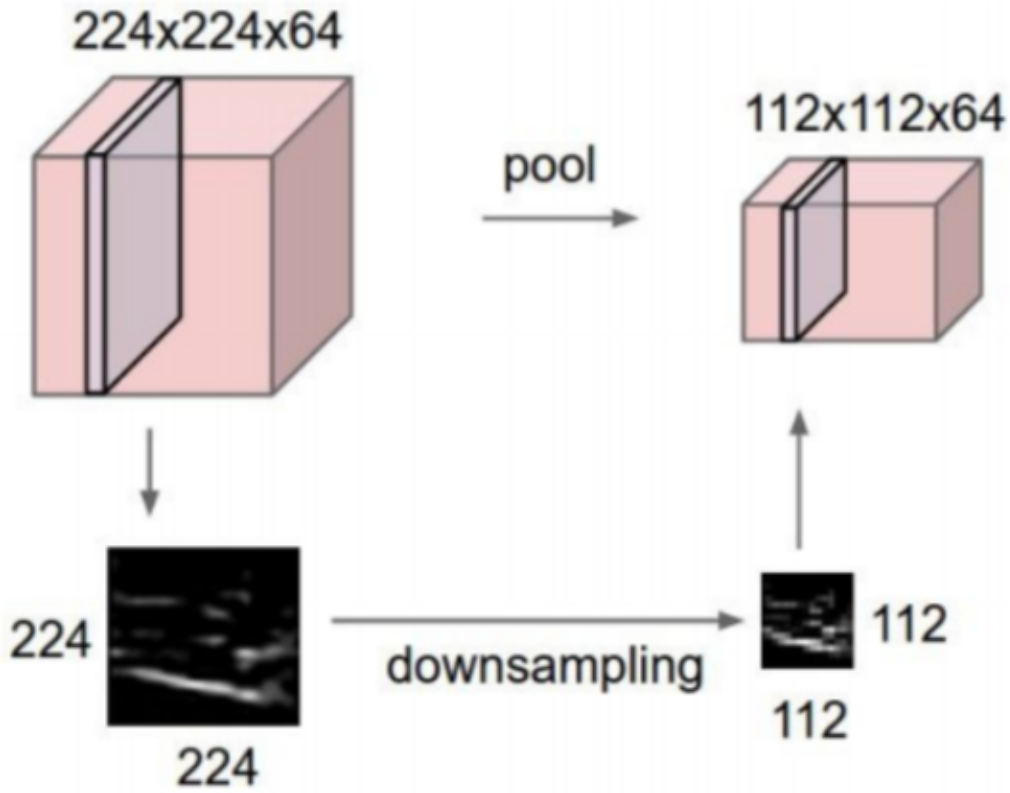
Pooling Layers

- makes the representations smaller and more manageable
- operates over each activation map independently:



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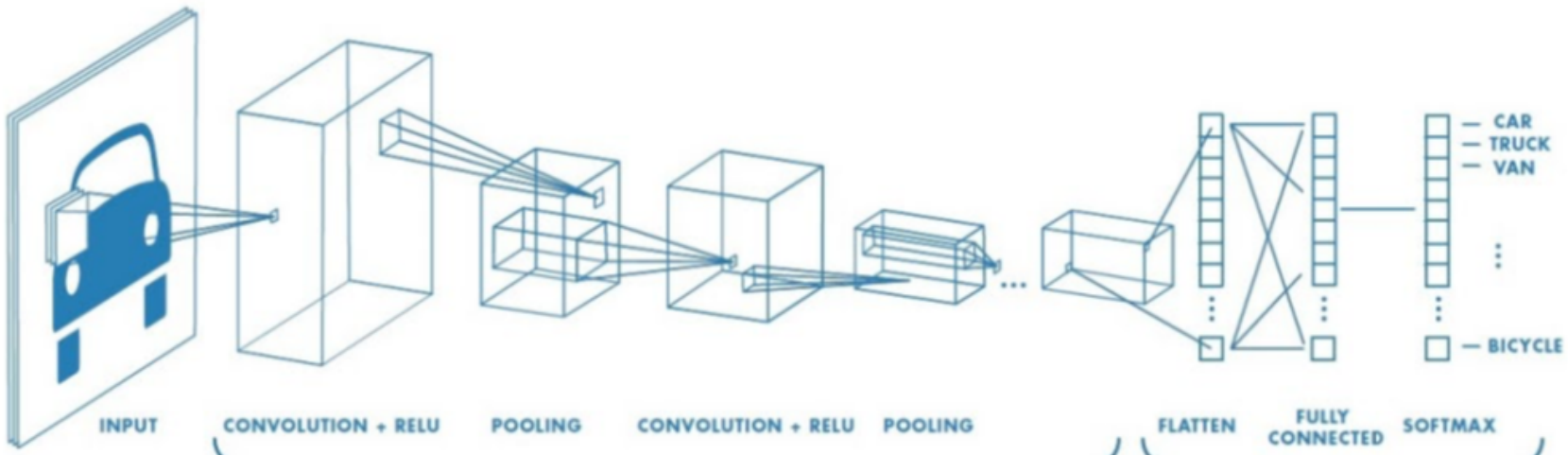
Flowchart of CNN



Learn weights for convolutional filters and fully connected layers

Backpropagation: cross-entropy loss

$$J(\boldsymbol{\theta}) = \sum_i y^{(i)} \log\left(\hat{\boldsymbol{y}}^{(i)}\right)$$

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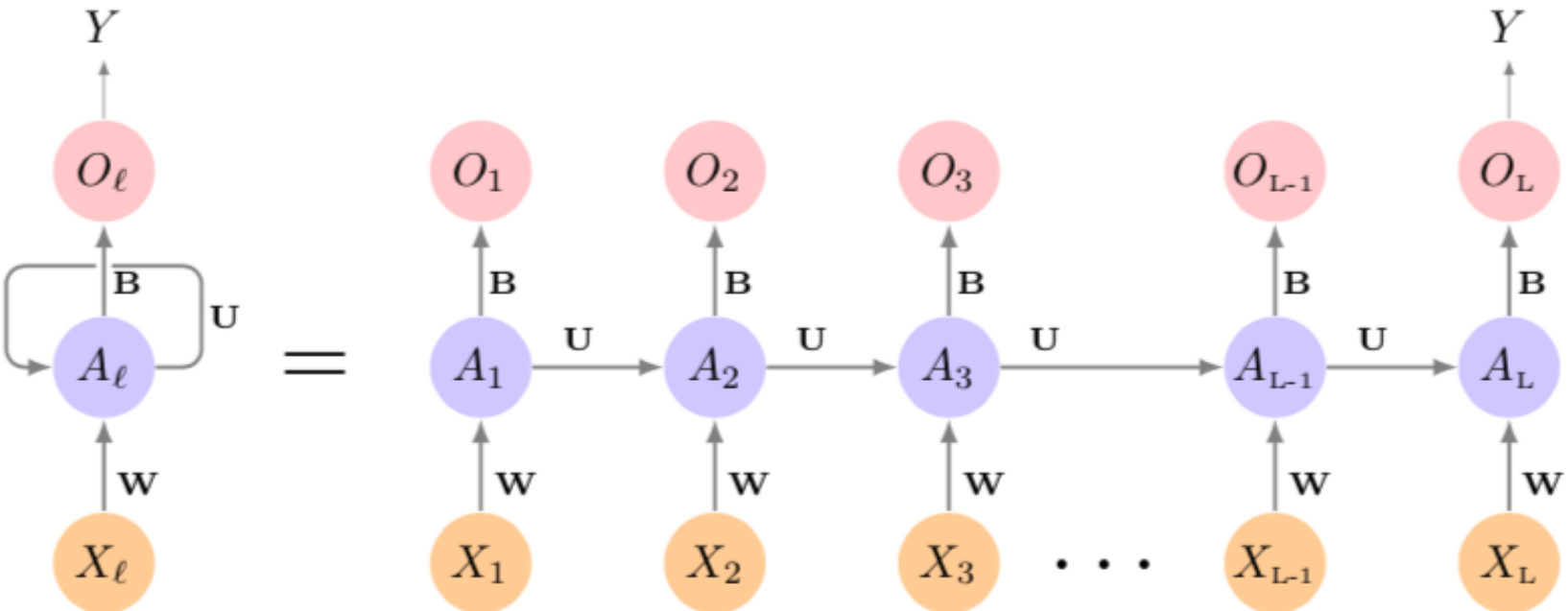
Recurrent Neural Network (RNN)

Motivation of RNN

RNN is designed for data being sequential in nature.

- Documents such as book and movie reviews, newspaper articles. The sequence of words can be exploited in tasks such as topic classification, sentiment analysis and language translation.
- Time Series of temperature, rainfall and so on. The aim is to forecast the weather several days ahead.
- Financial Time Series: market indices, trading volumes, stock and bond prices, and exchange rates. Accurate prediction is difficult for financial time series.
- Sound Recordings like recorded speech and musical recording. Aims may be to give a text transcription of a speech, or assess the quality of a piece of music.
- Handwriting, such as doctors' notes, and handwritten digits such as zip codes. Aim is to turn the handwriting into digital text, or read the digits.

Flowchart of RNN



Framework of RNN

- The input X is a sequence, i.e. $X = \{X_1, X_2, \ldots, X_L\}$. Each X_ℓ is a vector, i.e. $X_\ell = (X_{\ell 1}, X_{\ell 2}, \ldots, X_{\ell p})^\top$.
- The hidden layer consists of K units $A_\ell = (A_{\ell 1}, A_{\ell 2}, \ldots, A_{\ell K})^\top$.
- Input-layer Weights: $\mathbf{W} = (w_{kj})_{K\times(p+1)}$; Hidden-to-hidden layer weights: $\mathbf{U} = (u_{ks})_{K\times K}$; the output layer: $\mathbf{B} = (\beta_1, \beta_2, \ldots, \beta_{K+1})^\top$.
- The hidden layer: $A_{\ell k} = g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_{\ell j} + \sum_{s=1}^{K} u_{ks} A_{\ell-1,s}\right)$.
- The output O_ℓ is $O_\ell = \beta_0 + \sum_{k=1}^{K} \beta_k A_{\ell k}$.
- The loss function is $(Y - O_L)^2$.

Optimization in RNN

With n input sequence pairs (x_i, y_i), the shared parameters $\mathbf{W}, \mathbf{U}, \mathbf{B}$ are found by minimizing the sum of squares

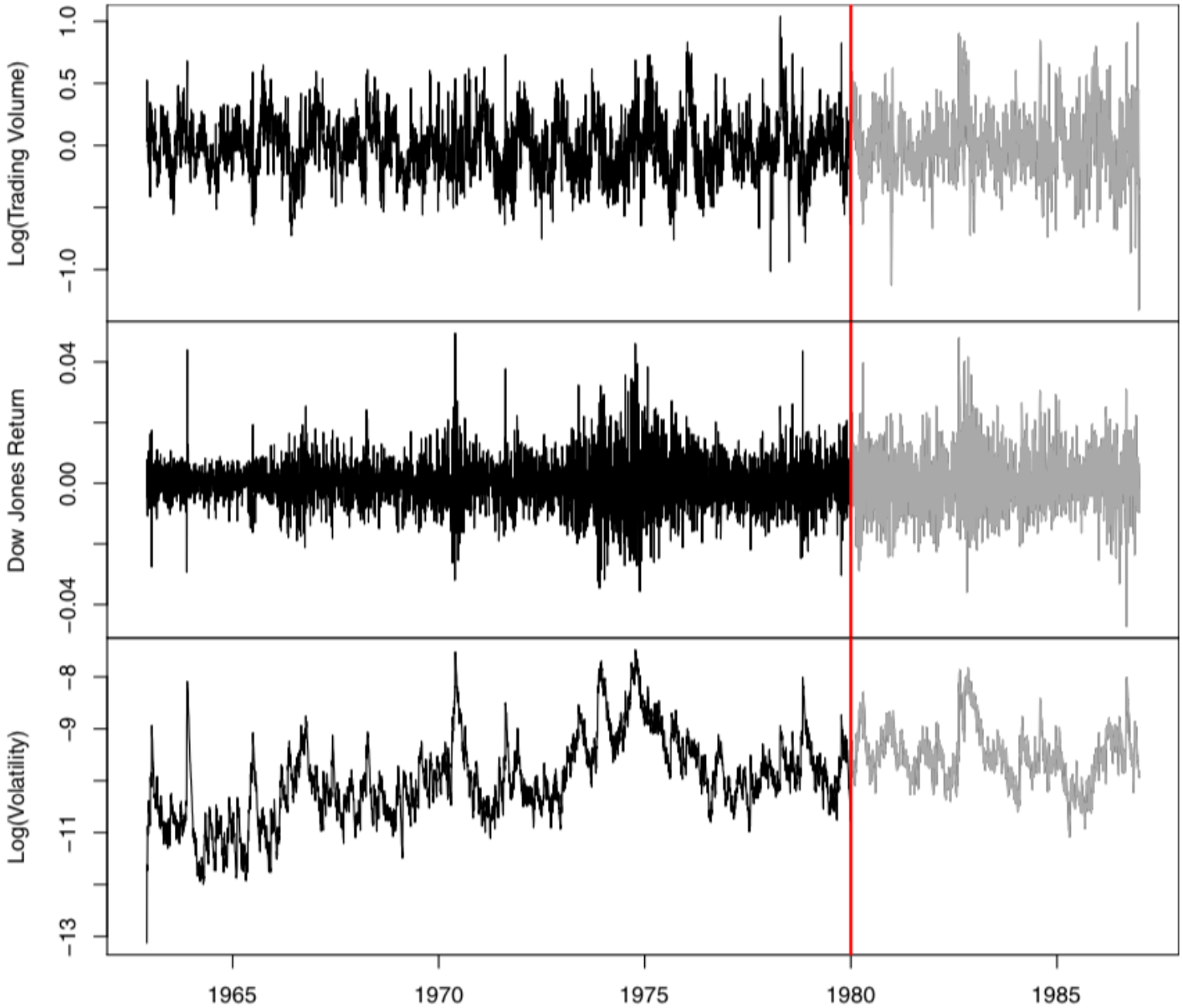
$$\sum_{i=1}^{n}(y_i - o_{iL})^2 = \sum_{i=1}^{n}\left(y_i - \left(\beta_0 + \sum_{k=1}^{K}\beta_k g\left(w_{k0} + \sum_{j=1}^{p} w_{kj}x_{iLj} + \sum_{s=1}^{K} u_{ks}a_{i,L-1,s}\right)\right)\right)^2.$$

Example: Financial Time Series Forecasting

Figure 10.14 shows historical trading statistics from the New York Stock Exchange. Shown are three daily time series covering the period December 3, 1962 to December 31, 1986:[19]

- `Log trading volume`. This is the fraction of all outstanding shares that are traded on that day, relative to a 100-day moving average of past turnover, on the log scale.
- `Dow Jones return`. This is the difference between the log of the Dow Jones Industrial Index on consecutive trading days.
- `Log volatility`. This is based on the absolute values of daily price movements.

Example: Financial Time Series Forecasting (Figure 10.14)



RNN Forecaster

- On day t, v_t: log trading volume; r_t: Dow Jones return; z_t: log volatility.
- Data: a total of $T = 6051$ such triples.
- Aim: to predict a value v_t from past values $v_{t-1}, v_{t-2}, \ldots$, and past values of the other series $r_{t-1}, r_{t-2}, \ldots$ and $z_{t-1}, z_{t-2}, \ldots$.
- The input sequence $X = \{X_1, X_2, \ldots, X_L\}$ and output Y are defined as follows.

$$X_1 = \begin{pmatrix} v_{t-L} \\ r_{t-L} \\ z_{t-L} \end{pmatrix}, \; X_2 = \begin{pmatrix} v_{t-L+1} \\ r_{t-L+1} \\ z_{t-L+1} \end{pmatrix}, \cdots, X_L = \begin{pmatrix} v_{t-1} \\ r_{t-1} \\ z_{t-1} \end{pmatrix}, \quad \text{and } Y = v_t.$$

- Here, $L = 5$, $K = 12$ hidden units using 4281 training data and then forecast the 1770 values of v_t. We achieve $R^2 = 0.42$. The baseline model can attain $R^2 = 0.18$.

Example: RNN Forecast

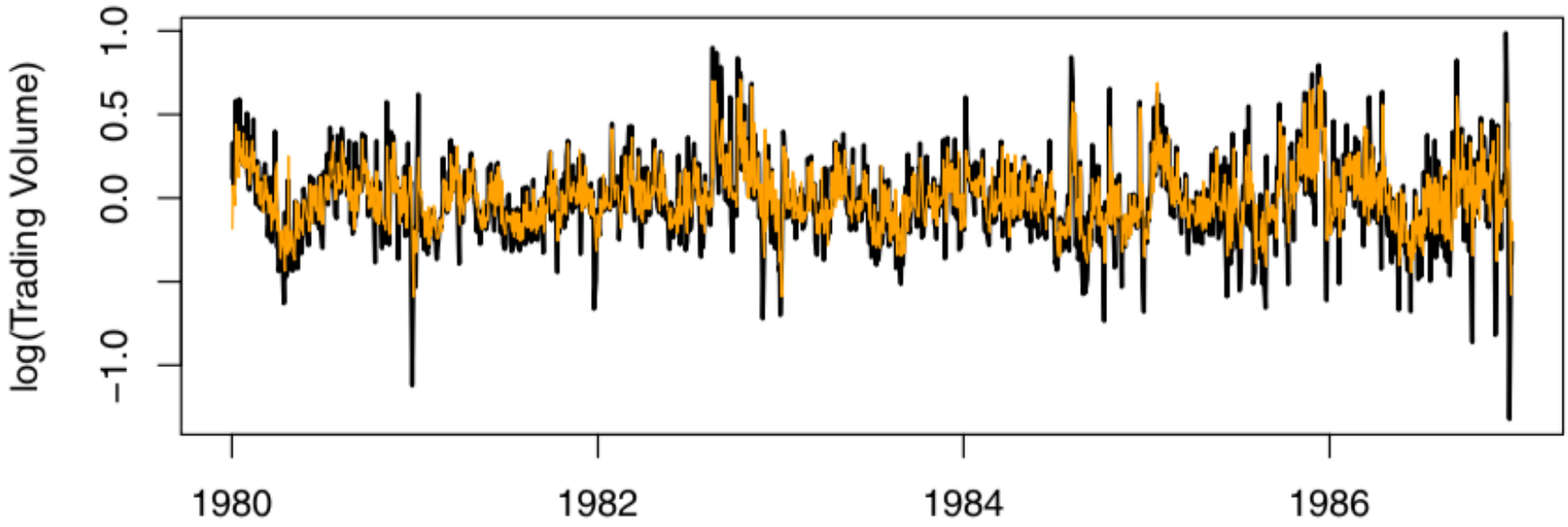
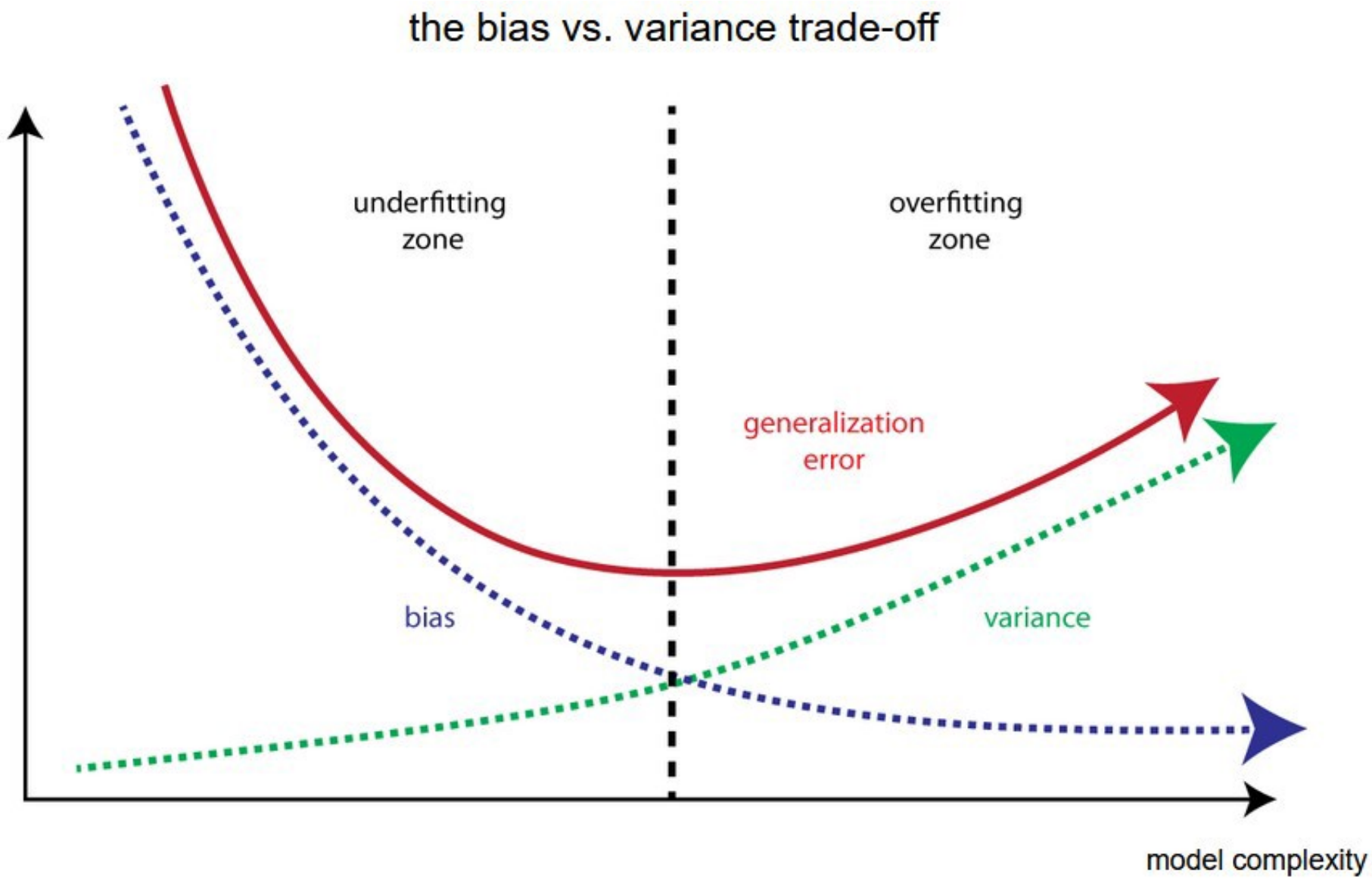


FIGURE 10.16. *RNN forecast of* `log_volume` *on the* `NYSE` *test data. The black lines are the true volumes, and the superimposed orange the forecasts. The forecasted series accounts for 42% of the variance of* `log_volume`.

Double Descent Phenomenon

Model Flexibility and Prediction Accuracy



Insights from Bias-Variance Tradeoff

- This trade-off indicates that statistical learning methods tend to perform the best, in terms of test error, for an intermediate level of model complexity.
- So one implication of the bias-variance trade-off is that it is generally not a good idea to interpolate the training data, that is, to get zero training error will result in very high test error.

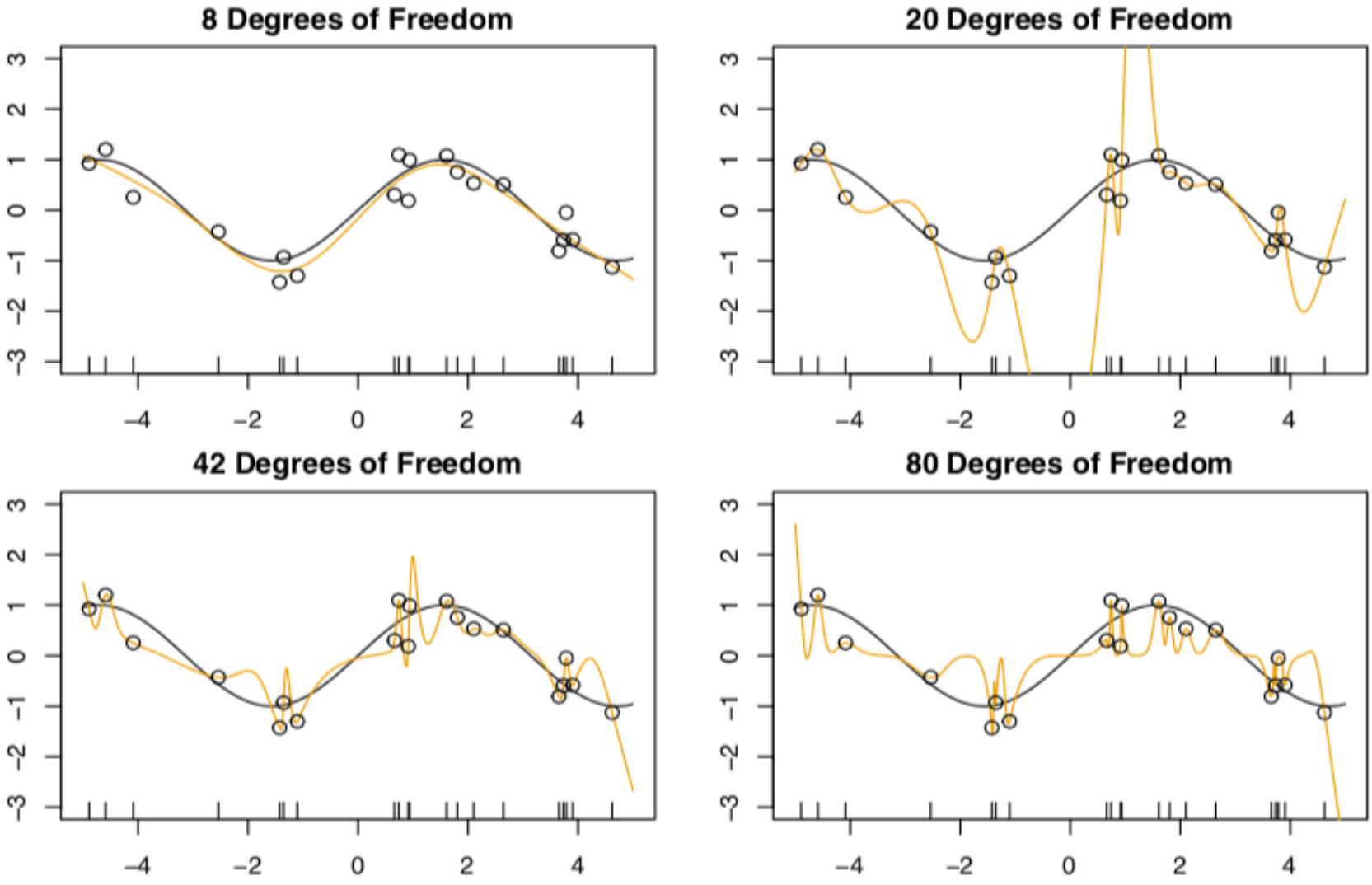
Example: Basis Expansion

- The regression model

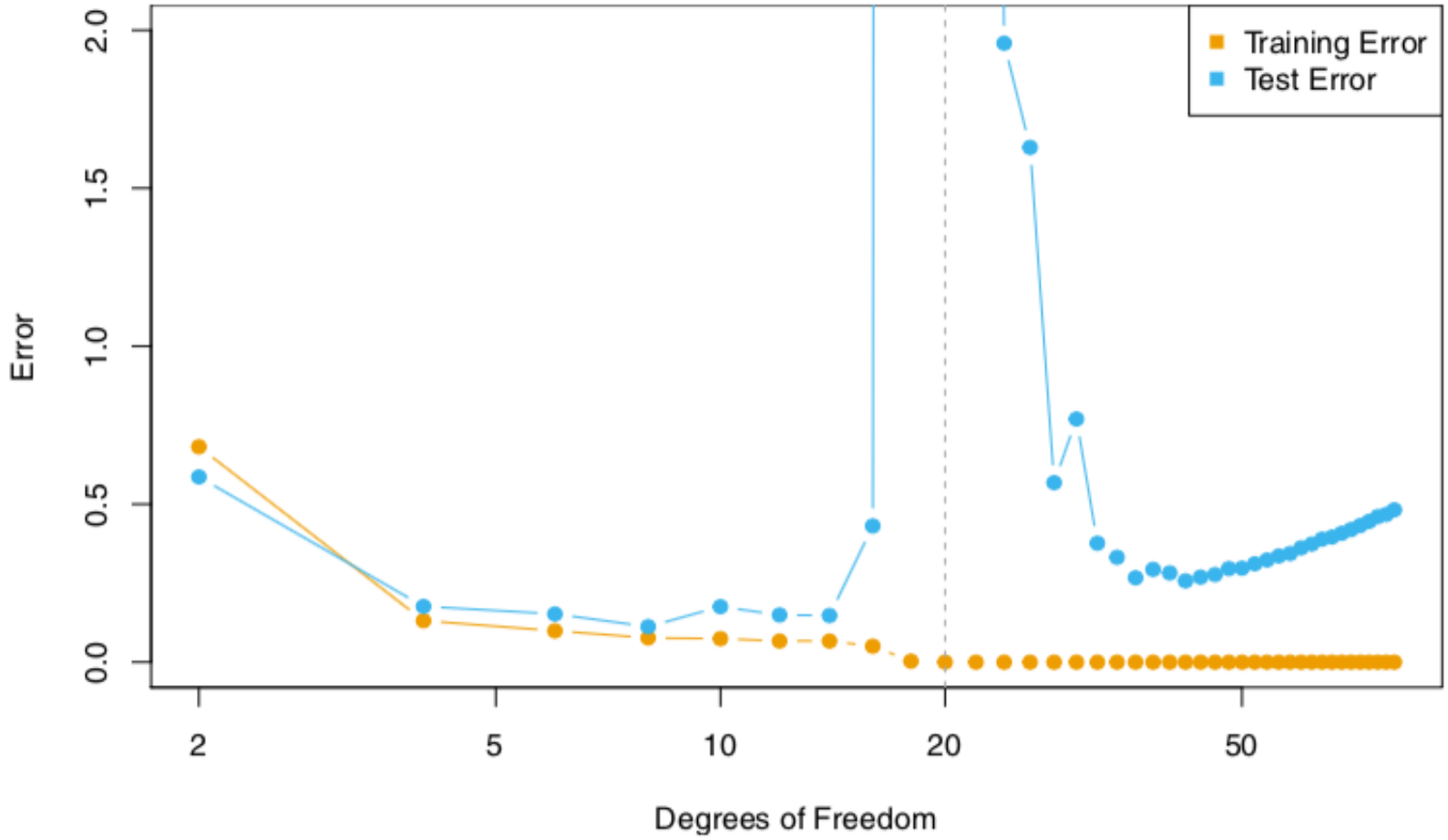
$$y_i = sin(x_i) + \varepsilon_i, \quad i = 1, 2, \ldots, n. \tag{8}$$

- The sample size $n = 20$.
- Predictors $x_i \sim U[-5, 5]$ and errors $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 0.3$.
- Fit a natural spline with d basis functions $B_\ell(x_i), \ell = 1, 2, \ldots, d$.
- The minimum-norm estimator for the linear coefficient in Basis Expansion is $\left(\mathbf{B}\mathbf{B}^\top\right)^- \mathbf{B}\mathbf{Y}$, where $\mathbf{B} = \left(B_\ell(x_i)\right)_{d \times n}$ and $\mathbf{Y} = (y_1, y_2, \ldots, y_n)^\top$.

Fitted Functions



Double Descent Phenomenon



Insights from Double Descent

- Interpolating the training data perform well, or at least, better than a slightly less complex model that does not quite interpolate the data.
- Double descent gets its name from the fact that the test error has a U-shape before the interpolation threshold is reached, and then it descends again as an increasingly flexible model is fit.
- The double descent phenomenon does not contradict the bias-variance trade-off.