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Deep Learning (Fall 2023)

Ikbeom Jang

ijang@hufs.ac.kr

CES HUFS

Linear Neural Networks

- Softmax Regression Implementation from Scratch
- Concise Implementation of Softmax Regression

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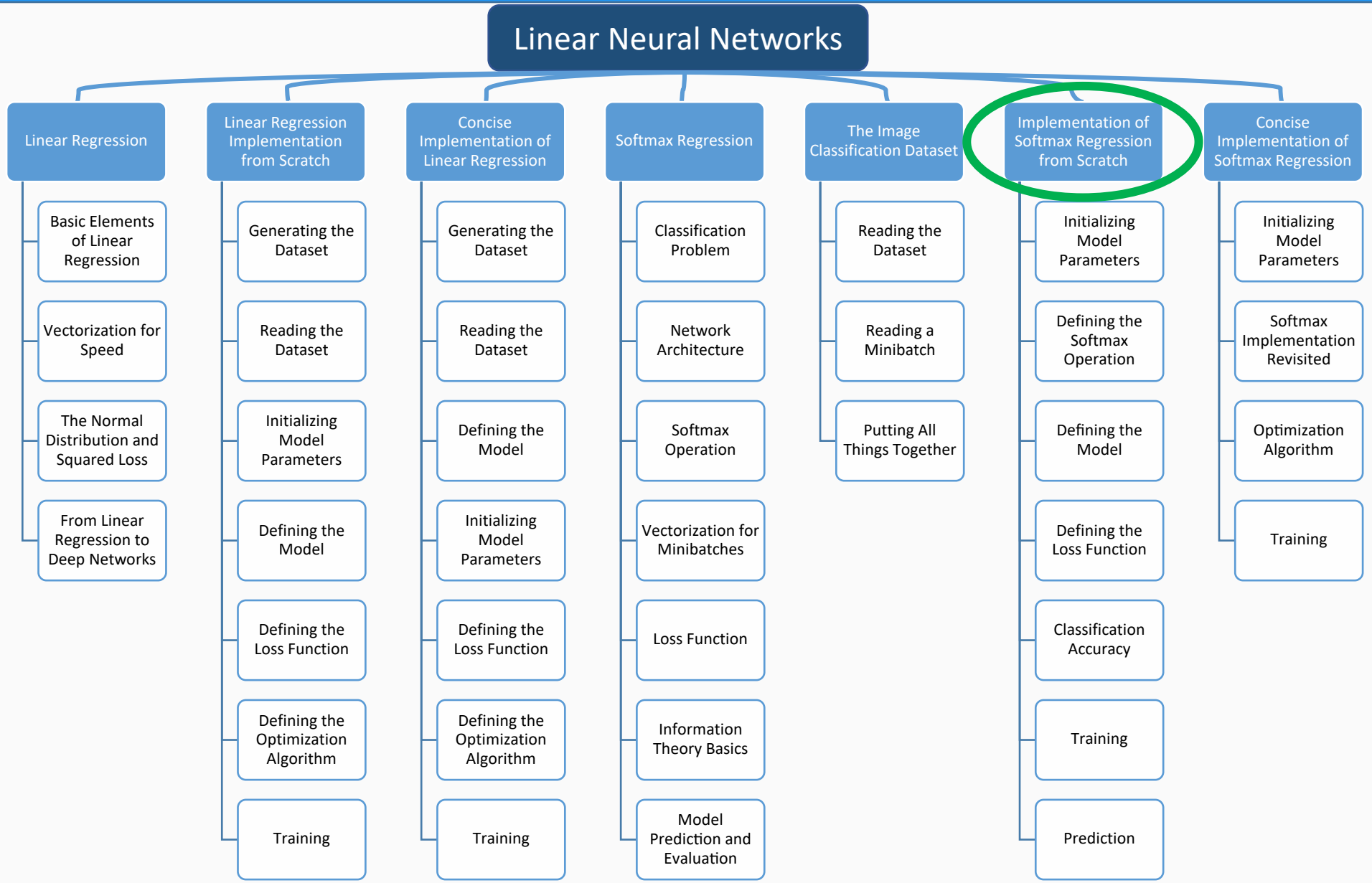
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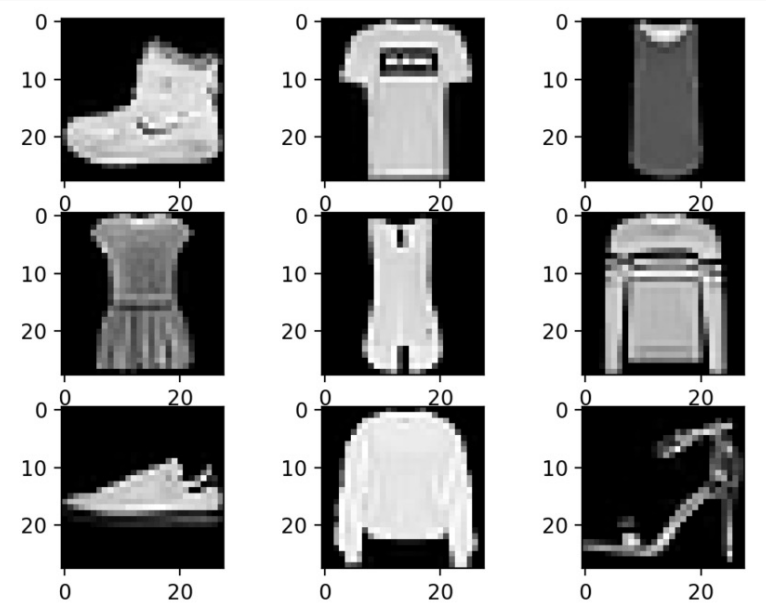
Softmax Regression Implementation from Scratch

- We focus on defining the softmax-specific aspects of the model.
- We reuse the other components from our linear regression section, including the training loop.
- We will use the Fashion-MNIST dataset.



```
import torch
from d2l import torch as d2l
```

The Softmax

- Let's start with the mapping from scalars to probabilities.
- Recall the operation of the sum operator along specific dimensions in a tensor
  - Given a matrix X we can sum over all elements (by default) or only over elements in the same axis.
  - The axis variable lets us compute row and column sums:

```
X = torch.tensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
X.sum(0, keepdims=True), X.sum(1, keepdims=True)
```

```
(tensor([[5., 7., 9.]]),
 tensor([[ 6.],
         [15.]]))
```

The Softmax

- Computing the softmax requires three steps:
  - (i) exponentiation of each term
  - (ii) a sum over each row to compute the normalization constant for each example
  - (iii) division of each row by its normalization constant, ensuring that the result sums to 1

$$\mathrm{softmax}(\mathbf{X})_{ij} = \frac{\exp(\mathbf{X}_{ij})}{\sum_k \exp(\mathbf{X}_{ik})}$$

- The (logarithm of the) denominator is called the (log) partition function.
  - It was introduced in statistical physics to sum over all possible states in a thermodynamic ensemble.

```
def softmax(X):
    X_exp = torch.exp(X)
    partition = X_exp.sum(1, keepdims=True)
    return X_exp / partition # The broadcasting mechanism is applied here
```

The Softmax

- For any input X, we turn each element into a non-negative number.
- Each row sums up to 1, as is required for a probability.
- Caution: the code above is not robust against very large or very small arguments.
  - While it is sufficient to illustrate what is happening, you should not use this code verbatim for any serious purpose.
  - Deep learning frameworks have such protections built in and we will be using the built-in softmax going forward.

```
X = torch.rand((2, 5))
X_prob = softmax(X)
X_prob, X_prob.sum(1)
```

```
(tensor([[0.2511, 0.1417, 0.1158, 0.2529, 0.2385],
         [0.2004, 0.1419, 0.1957, 0.2504, 0.2117]]),
 tensor([1., 1.]))
```

The Model

- We now have everything that we need to implement the softmax regression model.
- As in our linear regression example, each instance will be represented by a fixed-length vector.
- Since the raw data here consists of 28×28 pixel images, we flatten each image, treating them as vectors of length 784.
  - In later chapters, we will introduce convolutional neural networks, which exploit the spatial structure in a more satisfying way.

- In softmax regression, the number of outputs from our network should be equal to the number of classes.
- Since our dataset has 10 classes, our network has an output dimension of 10.
- Consequently, our weights constitute a 784×10 matrix plus a 1×10 row vector for the biases.
- As with linear regression, we initialize the weights W with Gaussian noise. The biases are initialized as zeros.

The Model

```
class SoftmaxRegressionScratch(d2l.Classifier):
    def __init__(self, num_inputs, num_outputs, lr, sigma=0.01):
        super().__init__()
        self.save_hyperparameters()
        self.W = torch.normal(0, sigma, size=(num_inputs, num_outputs), requires_grad=True)
        self.b = torch.zeros(num_outputs, requires_grad=True)

    def parameters(self):
        return [self.W, self.b]
```

- The code below defines how the network maps each input to an output.
- Note that we flatten each 28×28 pixel image in the batch into a vector using reshape before passing the data through our model.

```
@d2l.add_to_class(SoftmaxRegressionScratch)
def forward(self, X):
    X = X.reshape((-1, self.W.shape[0]))
    return softmax(torch.matmul(X, self.W) + self.b)
```

The Cross-Entropy Loss

- The cross-entropy loss is the most common loss function in all of deep learning.
  - At the moment, applications of deep learning easily cast as classification problems far outnumber those better treated as regression problems.

- Recall that cross-entropy takes the negative log-likelihood of the predicted probability assigned to the true label.

- For efficiency we avoid Python for-loops and use indexing instead.
  - In particular, the one-hot encoding in *y* allows us to select the matching terms in *y_hat*.

- To see this in action we create sample data *y_hat* with 2 examples of predicted probabilities over 3 classes and their corresponding labels *y*.
  - The correct labels are 0 and 2 respectively (i.e., the first and third class).
  - Using *y* as the indices of the probabilities in *y_hat*, we can pick out terms efficiently.

```
y = torch.tensor([0, 2])  # true labels (not one-hot encoded). It's [[1, 0, 0], [0,0,1]] if one-hot encoded.
y_hat = torch.tensor([[0.1, 0.3, 0.6], [0.3, 0.2, 0.5]])  # predicted labels
y_hat[[0, 1], y]  # for the 0th and 1st samples, choose the class in y_hat based on the true labels y
```

```
tensor([0.1000, 0.5000])
```

The Cross-Entropy Loss

- Recall the formula of cross-entropy loss:

$$l(y, \hat{y}) = -\sum_{j=1}^{q} y_j \log \hat{y}_j$$

- Now implement the cross-entropy loss function by averaging over the logarithms of the selected probabilities.
- Focus on "y_hat[list(range(len(y_hat))), y]" – it's tricky!!
  - What it does is: for all samples, choose the class in y_hat based on the true labels y (using indexing)
  - Choosing is equivalent to multiplying (in the equation) if you recall y are one-hot vectors like [0,0,1]

```
def cross_entropy(y_hat, y):
    return -torch.log(y_hat[list(range(len(y_hat))), y]).mean()

cross_entropy(y_hat, y)
```

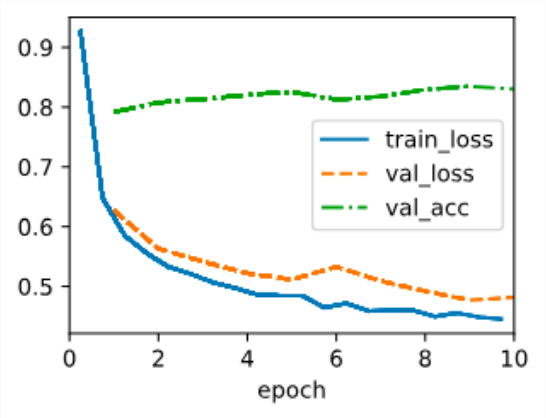
```
tensor(1.4979)
```

```
@d2l.add_to_class(SoftmaxRegressionScratch)
def loss(self, y_hat, y):
    return cross_entropy(y_hat, y)
```

Training

- We reuse the fit method defined in Section 3.4 to train the model with 10 epochs.
- Note that the number of epochs (max_epochs), the minibatch size (batch_size), and learning rate (lr) are adjustable hyperparameters.
  - That means that while these values are not learned during our primary training loop, they still influence the performance of our model, both in terms of training and generalization performance.
- In practice you will want to choose these values based on the validation split of the data and then, ultimately, to evaluate your final model on the test split.
  - We will regard the test data of Fashion-MNIST as the validation set, thus reporting validation loss and validation accuracy on this split.

```
data = d2l.FashionMNIST(batch_size=256)
model = SoftmaxRegressionScratch(num_inputs=784, num_outputs=10, lr=0.1)
trainer = d2l.Trainer(max_epochs=10)
trainer.fit(model, data)
```



Prediction

- Our model is ready to classify some images.

```
X, y = next(iter(data.val_dataloader()))
preds = model(X).argmax(axis=1)
preds.shape
```

```
torch.Size([256])
```

- We are usually more interested in the images we label incorrectly.
- We visualize them by comparing their actual labels (1st line of text output) with the model predictions (2nd line of text output).

```
wrong = preds.type(y.dtype) != y
X, y, preds = X[wrong], y[wrong], preds[wrong]
labels = [a+'\n'+b for a, b in zip(data.text_labels(y), data.text_labels(preds))]
data.visualize([X, y], labels=labels)
```

Summary

- By now we are starting to get some experience with solving linear regression and classification problems.
- With it, we have reached what would be the state of the art of 1960–1970s of statistical modeling.
- Next, we will learn how to leverage DL frameworks to implement this model much more efficiently.

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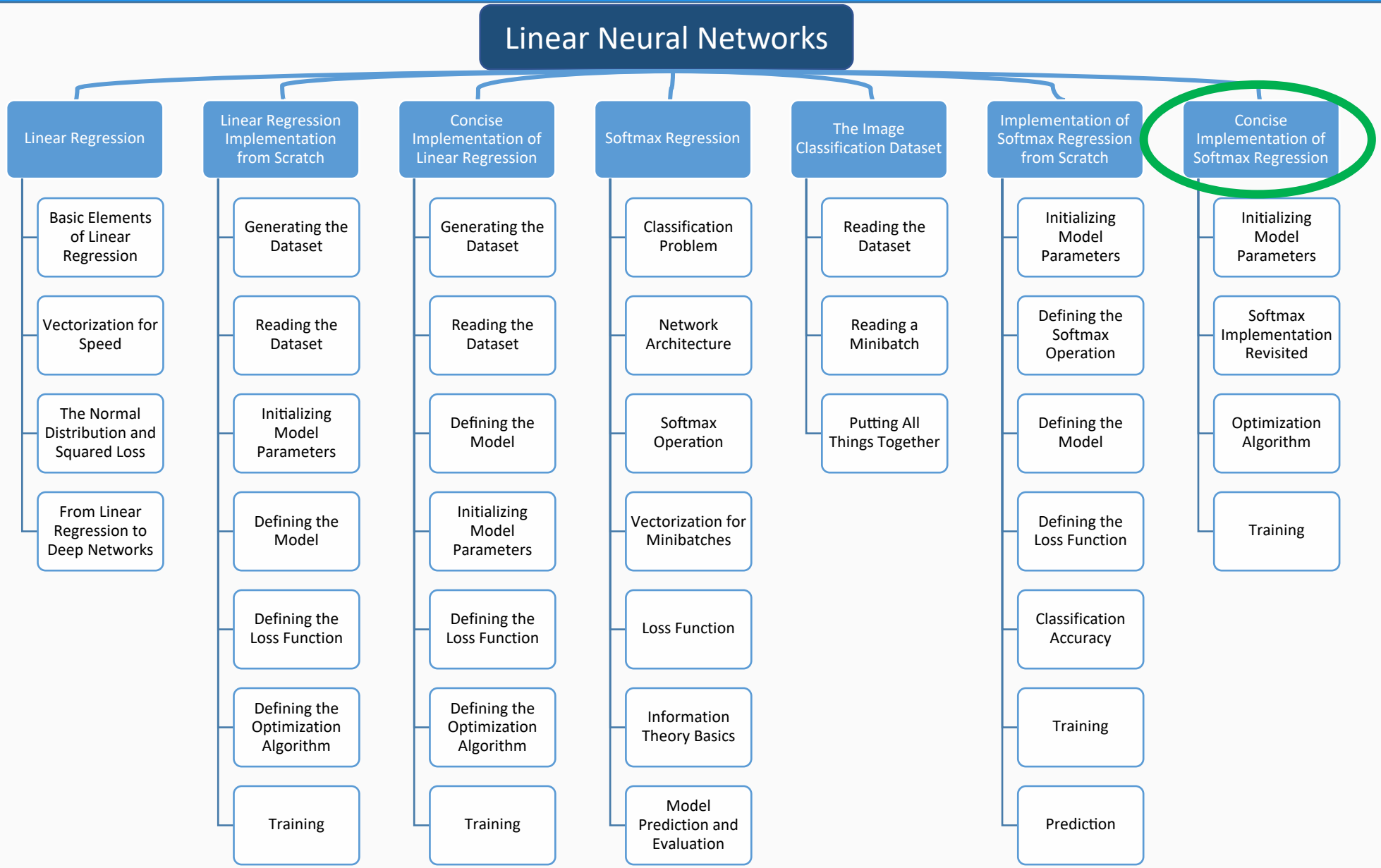
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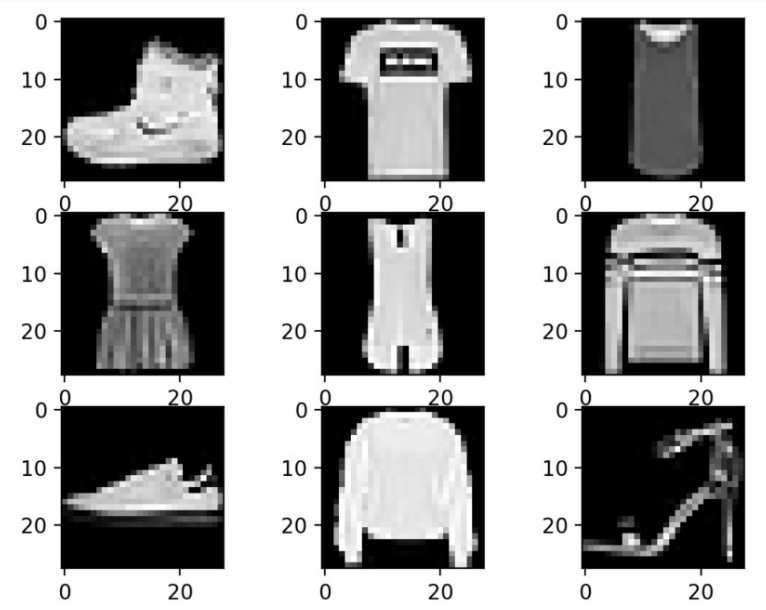
Concise Implementation of Softmax Regression

- Just as high-level DL frameworks made it easier to implement linear regression, they are similarly convenient here.



```
import torch
from torch import nn
from torch.nn import functional as F
from d2l import torch as d2l
```

Defining the Model

- We construct our fully connected layer using the built-in layer.
  - The built-in __call__ method then invokes forward whenever we need to apply the network to some input.

- We use a Flatten layer to convert the fourth-order tensor X to second order by keeping the dimensionality along the first axis unchanged.

```
class SoftmaxRegression(d2l.Classifier): #@save
    """The softmax regression model."""
    def __init__(self, num_outputs, lr):
        super().__init__()
        self.save_hyperparameters()
        self.net = nn.Sequential(nn.Flatten(), nn.LazyLinear(num_outputs))

    def forward(self, X):
        return self.net(X)
```

Softmax

- In the previous section, we calculated our model's output and applied the cross-entropy loss.
- While this is perfectly reasonable mathematically, it is risky computationally, because of numerical underflow and overflow in the exponentiation.
  - If some of the o_k are very large, then $exp(o_k)$ might be larger than the largest number we can have for certain data types. This is called overflow.
  - Likewise, if every argument is a very large negative number, we will get underflow.
  - For instance, single precision floating point numbers approximately cover the range of 10^{-38} to 10^{38}.
  - As such, if the largest term in $\boldsymbol{o}$ lies outside the interval [−90,90], the result will not be stable.
- A way round this problem is to subtract $\bar{o} \stackrel{\text{def}}{=} \max_k o_k$ from all entries (more explanation in textbook):

$$\hat{y}_j = \frac{\exp o_j}{\sum_k \exp o_k} = \frac{\exp(o_j - \bar{o}) \exp \bar{o}}{\sum_k \exp(o_k - \bar{o}) \exp \bar{o}} = \frac{\exp(o_j - \bar{o})}{\sum_k \exp(o_k - \bar{o})}$$

Softmax

- Fortunately, we are saved by the fact that even though we are computing exponential functions, we ultimately intend to take their log (when calculating the cross-entropy loss).
- By combining softmax and cross-entropy, we can escape the numerical stability issues altogether. We have:

$$\log \hat{y}_j = \log \frac{\exp(o_j - \bar{o})}{\sum_k \exp(o_k - \bar{o})} = o_j - \bar{o} - \log \sum_k \exp(o_k - \bar{o}).$$

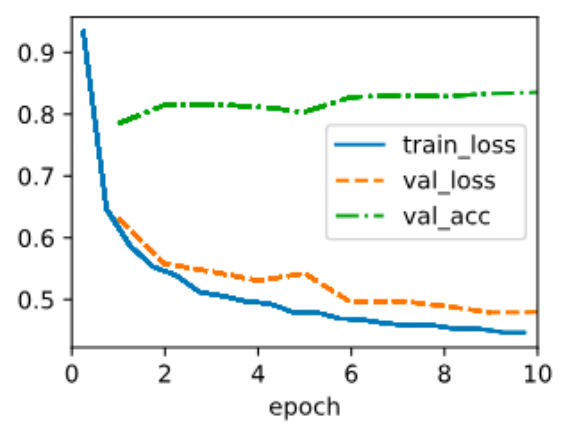
- This avoids both overflow and underflow.
- We will want to keep the conventional softmax function handy in case we ever want to evaluate the output probabilities by our model.
- But instead of passing softmax probabilities into our new loss function, we just pass the logits and compute the softmax and its log all at once inside the cross-entropy loss function.

```
@d2l.add_to_class(d2l.Classifier) #@save
def loss(self, Y_hat, Y, averaged=True):
    Y_hat = Y_hat.reshape((-1, Y_hat.shape[-1]))
    Y = Y.reshape((-1,))
    return F.cross_entropy(Y_hat, Y, reduction='mean' if averaged else 'none')
```

Training

- Next, we train our model.
- We use Fashion-MNIST images, flattened to 784-dimensional feature vectors.
- As before, this algorithm converges to a solution that is reasonably accurate

```
data = d2l.FashionMNIST(batch_size=256)
model = SoftmaxRegression(num_outputs=10, lr=0.1)
trainer = d2l.Trainer(max_epochs=10)
trainer.fit(model, data)
```



Summary

- High-level APIs are very convenient at hiding from their user potentially dangerous aspects, such as numerical stability.
- Moreover, they allow users to design models concisely with very few lines of code.
- This is both a blessing and a curse.
  - The benefit is that it makes things highly accessible, even to engineers who never took a single class of statistics in their life.
  - But hiding the sharp edges also comes with a price: a disincentive to add new and different components on your own, since there is little muscle memory for doing it.
  - Moreover, it makes it more difficult to fix things whenever the protective padding of a framework fails to cover all the corner cases entirely.
- As such, it is urged to review both the bare bones and the elegant versions of many of the implementations that follow.
- I hope you can build on these when you invent something new that no framework can give you.