Lecture 3: Multilayer Perceptions

Reading: Chapter 4.1-4.5 of *Dive Into Deep Learning*

Outline

- Multilayer fully connected neural networks
- Model Selection, overfitting and underfitting
- Regularisization methods: weight decay

Multilayer Perceptrons

Limitatios of Linear Models

- Assumption of *monotonicity*: outputs increase proportionally with any feature
- Limited capacity: can only separate linearly separable data.
    - A data set is linearly separable if for each class there is a hyperplane to separate this class from the others.
- To increse model capacity, one needs to introduce non-linear models

From Single Layer to Multiple Layers

- To overcome the limitations of linear models, one can introduce hidden layers and
- Stack many fully-connected layers on top of each other.

An MLP with a hidden layer of 5 hidden units.

- A composite function based on linear transformations: the output of each preceding layer is fed as the input of the following layer.
- However, a simple stacking of multiple linear transformations is still equivalent to another linear transformation.

  $z = A_1 x, y = A_2 z$, then $y = Bx$ where $B = A_2 A_1$

From Linear to Nonlinear

- *Activation function* σ is applied to each hidden unit following the linear transformation.
- With activation functions in place, it is no longer going to collapse our MLP into a linear model.

$$
\begin{aligned}
H &= \sigma(XW^{(1)} + b^{(1)}), \\
O &= HW^{(2)} + b^{(2)}.
\end{aligned}
$$

- To build more general MLPs, we can continue stacking such hidden layers:

$$H^{(1)} = \sigma_1(XW^{(1)} + b^{(1)}), H^{(2)} = \sigma_2(H^{(1)}W^{(2)} + b^{(2)})$$

Universal Approximators

- MLPs are universal approximators which means they can approximate any nonlinear functions.
- Even with a single-hidden-layer network, given enough nodes, and the right set of weights, one can model any function, though
    - learning that function may be difficult.
- Many functions can be approximately much more compactly by using deeper (vs. wider) networks.

Activation Functions

- Activation functions decide whether a neuron should be activated or not.

In [1]:

```
%matplotlib inline
import torch
from d2l import torch as d2l
```

ReLU Function

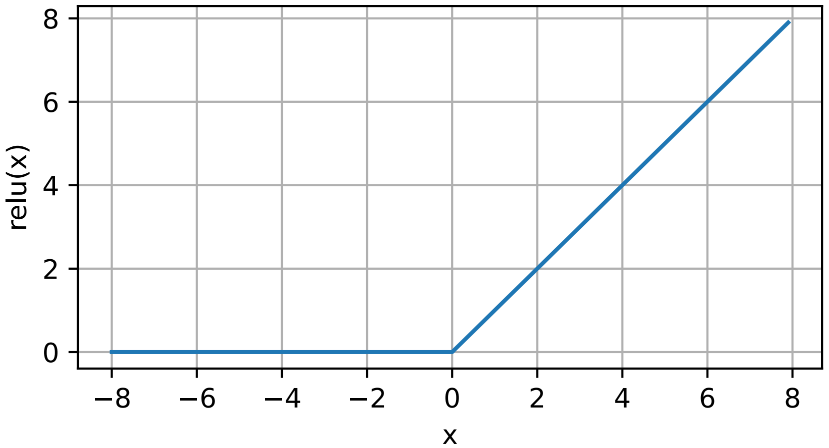
- *Rectified linear unit* (*ReLU*). Given an element x,

$$\mathrm{ReLU}(x) = \max(x, 0).$$

- The ReLU function retains only positive elements and discards all negative elements by setting the corresponding activations to 0.
- Piecewise linear

In [2]:

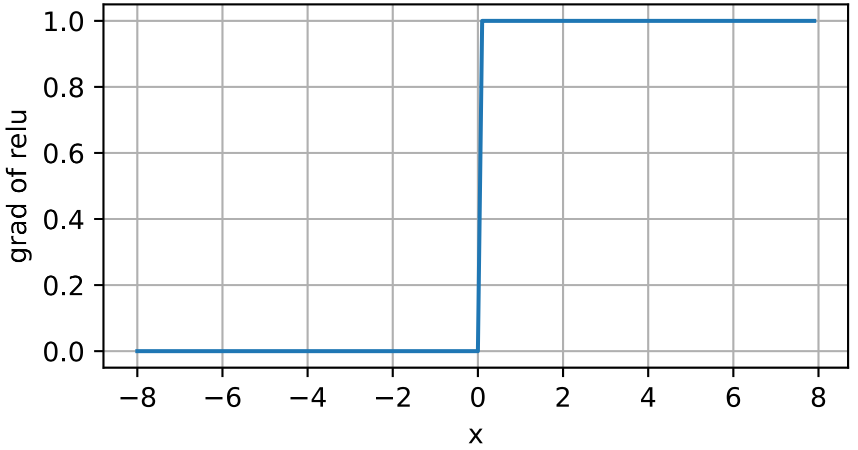
```
x = torch.arange(-8.0, 8.0, 0.1, requires_grad=True)
y = torch.relu(x)
d2l.plot(x.detach(), y.detach(), 'x', 'relu(x)', figsize=(5, 2.5))
```



- *Derivative* of the ReLU function: 0 when the input is negative, and 1 when the input is positive
- The ReLU function is not differentiable when the input is 0. In practice, we set the derivative as 0.

In [3]:

```
y.backward(torch.ones_like(x), retain_graph=True)
d2l.plot(x.detach(), x.grad, 'x', 'grad of relu', figsize=(5, 2.5))
```



- Variants: *parameterized ReLU* (*pReLU*) function

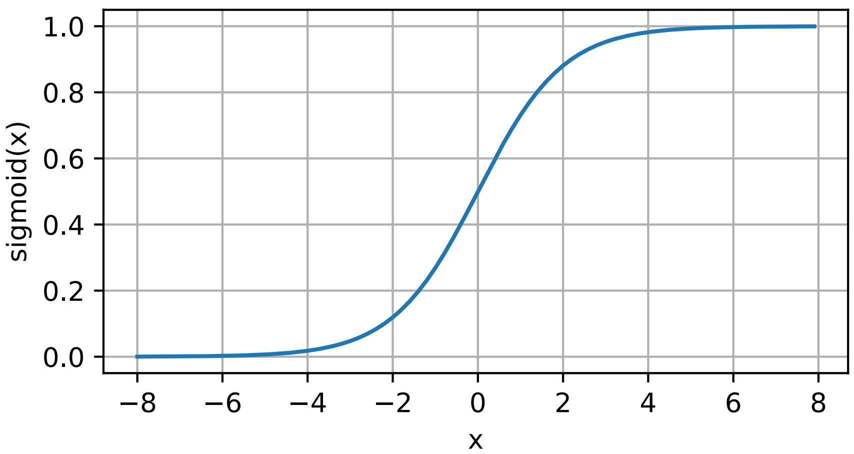
$$\mathrm{pReLU}(x) = \max(0, x) + \alpha \min(0, x).$$

Sigmoid Function

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}.$$

In [4]:

```
y = torch.sigmoid(x)
d2l.plot(x.detach(), y.detach(), 'x', 'sigmoid(x)', figsize=(5, 2.5))
```

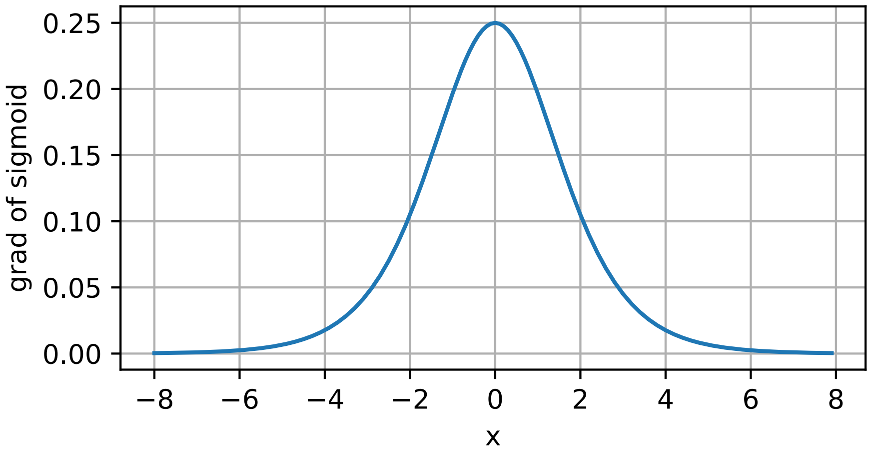


- The derivative of the sigmoid function:

$$\frac{d}{dx}\operatorname{sigmoid}(x) = \frac{\exp(-x)}{(1+\exp(-x))^2} = \operatorname{sigmoid}(x)\left(1-\operatorname{sigmoid}(x)\right).$$

In [5]:

```
# Clear out previous gradients
x.grad.data.zero_()
y.backward(torch.ones_like(x),retain_graph=True)
d2l.plot(x.detach(), x.grad, 'x', 'grad of sigmoid', figsize=(5, 2.5))
```

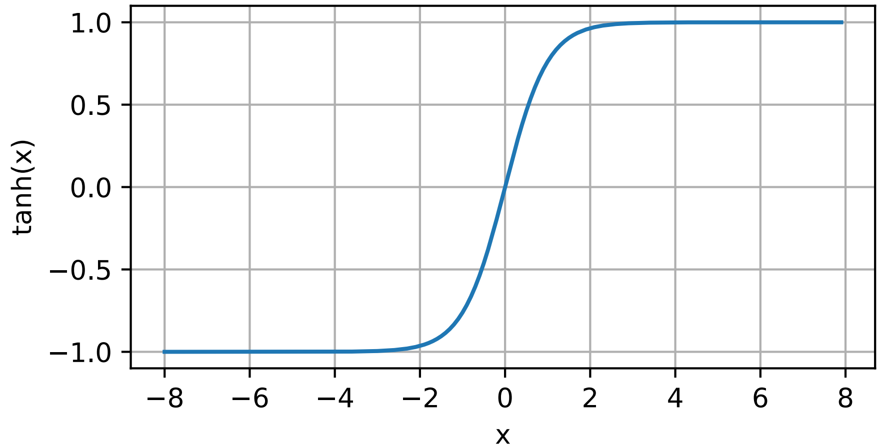


Tanh Function

$$\tanh(x) = \frac{1 - \exp(-2x)}{1 + \exp(-2x)}.$$

In [6]:

```
y = torch.tanh(x)
d2l.plot(x.detach(), y.detach(), 'x', 'tanh(x)', figsize=(5, 2.5))
```

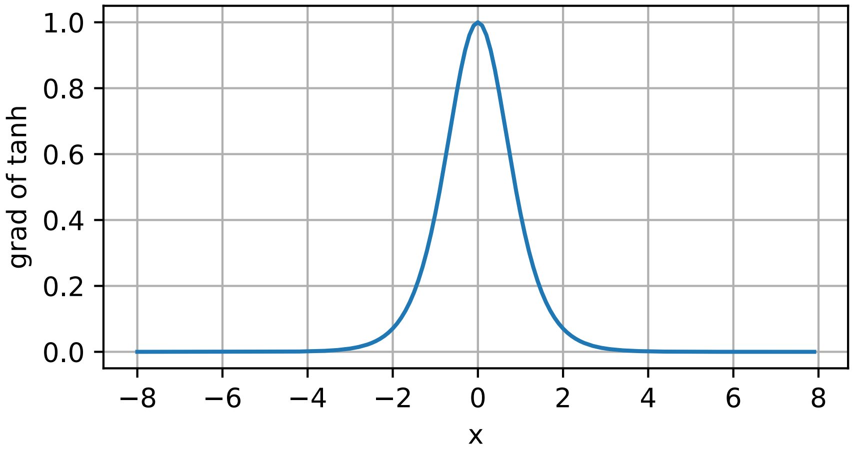


The derivative of the tanh function is:

$$\frac{d}{dx}\tanh(x) = 1 - \tanh^2(x).$$

In [7]:

```
# Clear out previous gradients.
x.grad.data.zero_()
y.backward(torch.ones_like(x),retain_graph=True)
d2l.plot(x.detach(), x.grad, 'x', 'grad of tanh', figsize=(5, 2.5))
```



Summary

- MLP adds one or multiple fully-connected hidden layers between the output and input layers and transforms the output of the hidden layer via an activation function.
- Commonly-used activation functions include the ReLU function, the sigmoid function, and the tanh function. With each of these activation functions, MLPs with a single hidden layer is a universal approximator.

Implementation of Multilayer Perceptrons

In [8]:

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

Model

- Input dimension: 784
- Output dimension: 10
- Hidden layer dimension: 256

In [9]:

```
net = nn.Sequential(nn.Flatten(),
                    nn.Linear(784, 256),
                    nn.ReLU(),
                    nn.Linear(256, 10))

def init_weights(m):
    if type(m) == nn.Linear:
        nn.init.normal_(m.weight, std=0.01)

net.apply(init_weights);
```

Training

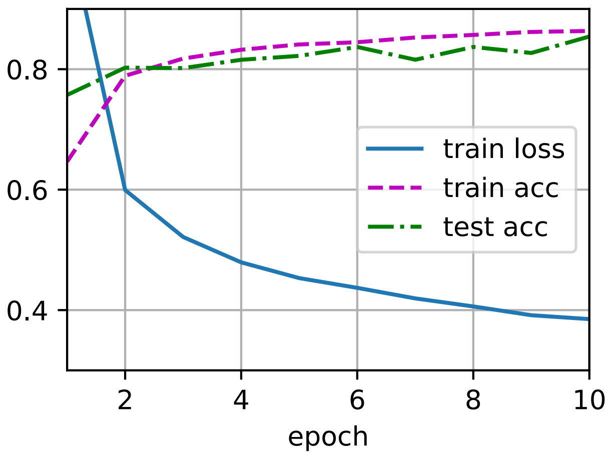
- Similar to Softmax regression

In [10]:

```
batch_size, lr, num_epochs = 256, 0.1, 10
loss = nn.CrossEntropyLoss()
trainer = torch.optim.SGD(net.parameters(), lr=lr)
```

In [11]:

```
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
d2l.train_ch3(net, train_iter, test_iter, loss, num_epochs, trainer)
```



Underfitting, Overfitting and Model Selection,

- The goal of machine learning is to discover patterns that *generalize* from training data to unseen data
- In learning of the models, we rely on the training data only
- Training data is a usually a small sample of the data with some underlying distribution
- Overfitting: the danger to fit the training data well but fail to generalize
- Regularisation: techniques to combat overfitting

- Models usually involve some hyperparameters.
  - Hyperparameters: the parameters which define the learning framework
  - Parameter of the model: the parameters which define a model in a general learning framework
  - Weights of linear regression or neural networks are parameters
  - Learning rate, epoch number, regularization number, number of neurons are hyper-parameters

- In practice, one often split the available data into subsets: training set and validation set.
    - The training set is used to learn the parameters of the model
    - The validation set is used to select the hyper-parameters.

Training Error and Generalization Error

- The *training error* is the error of our model as calculated on the training dataset,
- *Generalization error* is the expectation of our model's error when we apply the model to an infinite stream of additional data examples drawn from the same underlying data distribution as our original sample.
- We can never calculate the generalization error exactly.
- We must *estimate* the generalization error by applying our model to an independent test set.

Statistical Learning Theory

- *i.i.d. assumption*: both the training data and the test data are drawn *independently* from *identical* distributions.
- The model complexity affects the generalization performance: VC dimension
- Simple models and abundant data: we expect the generalization error to resemble the training error.
- Difficult to compare the complexity among different model classes

Common factors of generalization

1. The number of tunable parameters.
2. The values taken by the parameters. When weights can take a wider range of values, models can be more susceptible to overfitting.
3. The number of training examples.

Model Selection

- Model selection: the process to select the model after evaluating several candidate models.
- A validation dataset is used if a large amount of data is available.
- Use cross-validation if the data size is small.

K-Fold Cross-Validation

- The original training data is split into K non-overlapping subsets.
- Then model training and validation are executed K times,
- each time training on $K - 1$ subsets and validating on a different subset (the one not used for training in that round).
- Finally, the training and validation errors are estimated by averaging over the results from the K experiments.

Underfitting or Overfitting?

- Generalization gap: the difference between the training error and the validation error
- Underfitting: substantial training error, small generalization gap
    - The model is usually too simple to reduce the training error
- Overfitting: small training error, large generalization gap
- Factors: the complexity of the model and the size of the available training datasets.

Model Complexity

- An illustrative example: the polynomial of degree d

$$\hat{y} = \sum_{i=0}^{d} x^i w_i$$

- Treat x^i as a feature for each i.
- Then this is just a linear regression problem

- A higher-order polynomial function is more complex than a lower-order polynomial function.
- The relationship between polynomial degree and underfitting vs. overfitting

  Influence of model complexity on underfitting and overfitting

Weight Decay

- A simple regularization method
- Use norms of the weight vector to measure the complexity of the linear model
- Add its norm as a penalty term in the loss function

- Least squared errors

$$L(w, b) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{2}\left(w^\top x^{(i)} + b - y^{(i)}\right)^2.$$

- Least squared error plus L_2 norm penalty: ridge regression

$$L(w, b) + \frac{\lambda}{2}\|w\|^2,$$

- $\lambda = 0$: reduces to the least sqaured error function.
- $\lambda > 0$, restricts the size of $\|w\|$.
- Divide by 2: convention. when we take the derivative of a quadratic function, the 2 and $1/2$ cancel out, ensuring that the expression for the update looks nice and simple.

- One can also use other types of norms in the penalty terms
  - L_1 norm: LASSO (least absolute shrinkage and selection operator)

$$L(w, b) + \lambda \|w\|_1^2$$

  - Combination of L_1 and L_2 norm: Elastic net regularization

$$L(w, b) + \frac{\lambda_2}{2} \|w\|^2 + \lambda_1 \|w\|_1^2$$

Implementation

- The minibatch stochastic gradient descent updates for L_2-regularized regression follow:

$$\mathbf{w} \leftarrow (1-\eta\lambda)\,\mathbf{w} - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \mathbf{x}^{(i)} \left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - y^{(i)}\right).$$

- Why called "weight decay"? Given the penalty term alone, the optimization algorithm *decays* the weight at each step of training.

High-Dimensional Linear Regression

- Illustrate the benefits of weight decay through a simple synthetic example.

In [12]:

```
%matplotlib inline
import torch
from torch import nn
from d2l import torch as d2l
```

Data generation

$$y = 0.05 + \sum_{i=1}^{d} 0.01 x_i + \epsilon \text{ where } \epsilon \sim N(0, 0.01^2).$$

- The label is a linear function of our inputs,
- corrupted by Gaussian noise with zero mean and standard deviation 0.01.
- High dimension $d = 200$
- Small number of training example: 20 examples.

In [13]:

```
n_train, n_test, num_inputs, batch_size = 20, 100, 200, 5
true_w, true_b = torch.ones((num_inputs, 1)) * 0.01, 0.05
train_data = d2l.synthetic_data(true_w, true_b, n_train)
train_iter = d2l.load_array(train_data, batch_size)
test_data = d2l.synthetic_data(true_w, true_b, n_test)
test_iter = d2l.load_array(test_data, batch_size, is_train=False)
```

Implementation from Scratch

[**Initializing Model Parameters**]

- Randomly initialize the model parameters.

In [14]:

```
def init_params():
    w = torch.normal(0, 1, size=(num_inputs, 1), requires_grad=True)
    b = torch.zeros(1, requires_grad=True)
    return [w, b]
```

(Defining L_2 Norm Penalty)

- Square all terms in place and sum them up.

In [15]:

```
def l2_penalty(w):
    return torch.sum(w.pow(2)) / 2
```

[Defining the Training Loop]

- First fits the model on the training set and
- evaluates it on the test set.
- The linear network and the squared loss are the same as linear regression
- The only change here is that our loss now includes the penalty term.

In [16]:

```
def train(lambd):
    w, b = init_params()
    net, loss = lambda X: d2l.linreg(X, w, b), d2l.squared_loss
    num_epochs, lr = 100, 0.003
    animator = d2l.Animator(xlabel='epochs', ylabel='loss', yscale='log',
                            xlim=[5, num_epochs], legend=['train', 'test'])
    for epoch in range(num_epochs):
        for X, y in train_iter:
            # The L2 norm penalty term has been added, and broadcasting
            # makes `l2_penalty(w)` a vector whose length is `batch_size`
            l = loss(net(X), y) + lambd * l2_penalty(w)
            l.sum().backward()
            d2l.sgd([w, b], lr, batch_size)
        if (epoch + 1) % 5 == 0:
            animator.add(epoch + 1, (d2l.evaluate_loss(net, train_iter, loss),
                                     d2l.evaluate_loss(net, test_iter, loss)))
    print('L2 norm of w:', torch.norm(w).item())
```

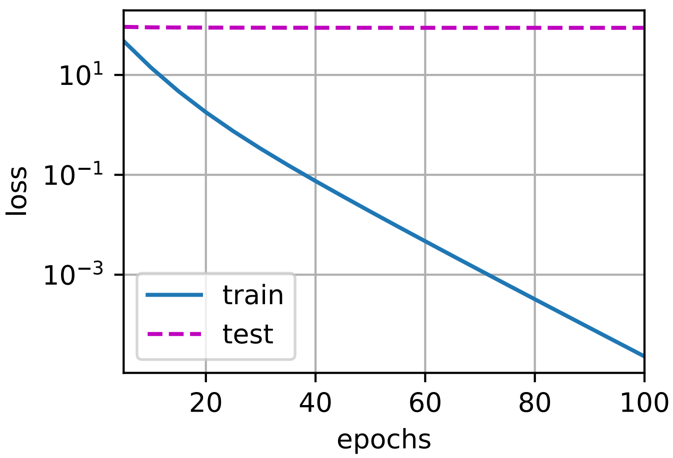
[Training without Regularization]

- Run this code with `lambd = 0`, disabling weight decay.

In [17]:

```
train(lambd=0)
```

```
L2 norm of w: 13.285733222961426
```



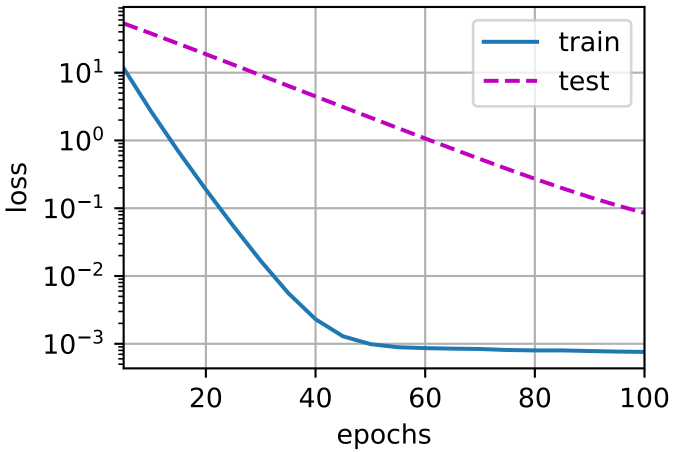
[Using Weight Decay]

- $\lambda = 3$: substantial weight decay.
- Training error increases
- but the test error decreases.

In [18]:

```
train(lambd=3)
```

```
L2 norm of w: 0.377597838640213
```



[Concise Implementation]

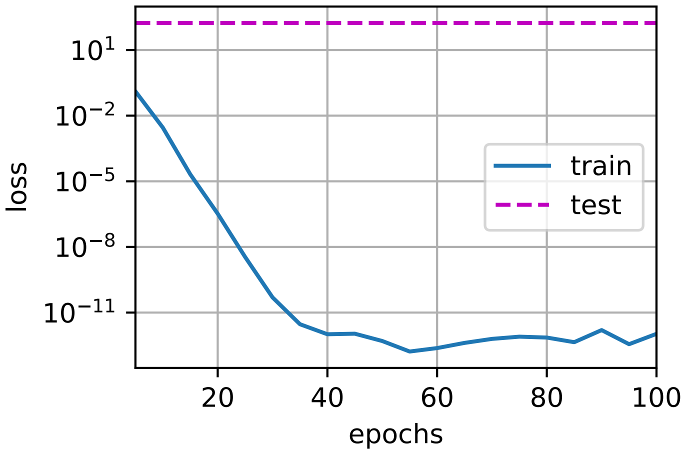
In [19]:

```
def train_concise(wd):
    net = nn.Sequential(nn.Linear(num_inputs, 1))
    for param in net.parameters():
        param.data.normal_()
    loss = nn.MSELoss(reduction='none')
    num_epochs, lr = 100, 0.003
    # The bias parameter has not decayed
    trainer = torch.optim.SGD([
        {"params":net[0].weight,'weight_decay': wd},
        {"params":net[0].bias}], lr=lr)
    animator = d2l.Animator(xlabel='epochs', ylabel='loss', yscale='log',
                            xlim=[5, num_epochs], legend=['train', 'test'])
    for epoch in range(num_epochs):
        for X, y in train_iter:
            trainer.zero_grad()
            l = loss(net(X), y)
            l.sum().backward()
            trainer.step()
        if (epoch + 1) % 5 == 0:
            animator.add(epoch + 1, (d2l.evaluate_loss(net, train_iter, loss),
                                     d2l.evaluate_loss(net, test_iter, loss)))
    print('L2 norm of w:', net[0].weight.norm().item())
```

In [20]:

```
train_concise(0)
```

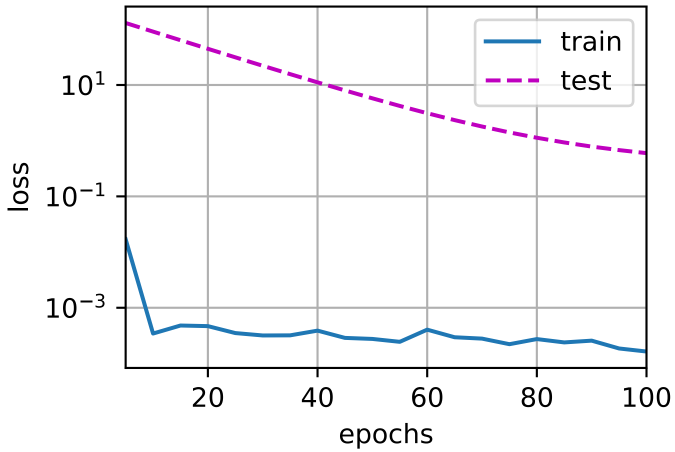
```
L2 norm of w: 13.32697868347168
```



In [21]:

```
train_concise(3)
```

```
L2 norm of w: 0.4191089868545532
```



Summary

- Regularization is a common method for dealing with overfitting. It adds a penalty term to the loss function on the training set to reduce the complexity of the learned model.
- One particular choice for keeping the model simple is weight decay using an L_2 penalty. This leads to weight decay in the update steps of the learning algorithm.