In [1]:
```
import numpy as np
import torch as t
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
%matplotlib inline
from ipywidgets import FloatSlider, IntSlider, interact, interact_m
anual
```

Part 3: Overfitting, regularisation and cross-validation

Varieties of overfitting

Too little data

If we have too little data, then our inferences can be very wrong, even with a simple model.

In [2]:
```
def bias(X):
    return t.cat([X, t.ones(X.shape[0], 1)], 1)
def fit_Wh(X, Y):
    return t.inverse(X.T @ X) @ X.T @ Y

def plot():
    N     = 3   # number of datapoints
    D     = 1   # dimension of datapoints
    sigma = 0.5 # output noise
    X     = t.tensor([[-0.1], [0], [0.1]])
    Xe    = bias(X)
    Wtrue = t.tensor([[2.], [-1]])
    Y     = Xe @ Wtrue + sigma*t.randn(N, 1)
    Wh    = fit_Wh(Xe, Y)

    fig, ax = plt.subplots()
    ax.set_xlabel("$x_\lambda$")
    ax.set_ylabel("$y_\lambda$")
    ax.set_xlim(-4, 4)
    ax.set_ylim(-4, 4)
    ax.scatter(X, Y, label="data");

    xs = t.linspace(-4, 4, 100)[:, None]
    ax.plot(xs, bias(xs)@Wtrue, 'b', label="true line")
    ax.plot(xs, bias(xs)@Wh, 'r', label="fitted")
    ax.legend()

interact_manual(plot);
```

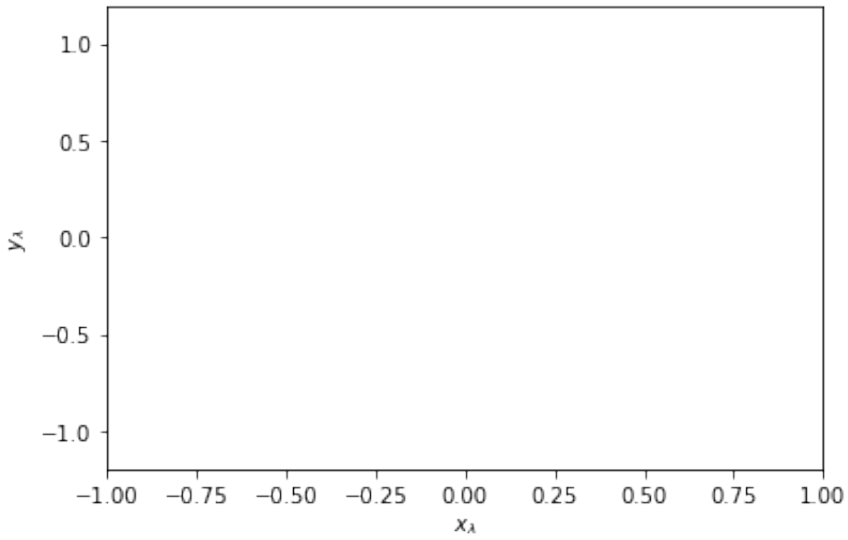
Too little data in some directions

In [4]:
```
def plot():
    N     = 100   # number of datapoints
    D     = 2   # dimension of datapoints
    sigma = 0.5 # output noise
    rand = t.randn(N, 1)
    X     = t.cat([rand, -rand], 1) + 1E-3*t.randn(N, 2)
    Wtrue = t.tensor([[1.], [-1.]])
    Y     = X @ Wtrue + sigma*t.randn(N, 1)
    Wh    = fit_Wh(X, Y)

    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.set_xlabel("$x_{\lambda, 0}$")
    ax.set_ylabel("$x_{\lambda, 1}$")
    ax.set_zlabel("$y_{\lambda, 0}$")
    ax.set_xlim(-4, 4)
    ax.set_ylim(-4, 4)
    ax.set_zlim(-15, 15)
    ax.scatter(X[:, 0], X[:, 1], Y[:, 0])

    Xp = t.tensor([
        [-4., -4.],
        [-4.,  4.],
        [ 4., -4.],
        [ 4.,  4.]
    ])

    ax.plot_trisurf(
        np.array(Xp[:, 0]),
        np.array(Xp[:, 1]),
        np.array((Xp @ Wh)[:, 0]),
        color='r',
        alpha=0.3
    )

interact_manual(plot);
```

The function class is too complex

For the sake of argument, we consider "Chebyshev polynomials". These are defined on $-1 \leq x \leq 1$ and range from $-1 \leq y \leq 1$,

In [5]:
```
def cheb(xs, c):
    # c is int
    coefs = c*[0] + [1]
    return np.polynomial.chebyshev.chebval(xs, coefs)

xs = np.linspace(-1, 1, 100)

fig, ax = plt.subplots()
ax.set_xlabel("$x_\lambda$")
ax.set_ylabel("$y_\lambda$")
ax.set_xlim(-1, 1)
ax.set_ylim(-1.2, 1.2)

i = 0
def add_line():
    global i
    ax.plot(xs, cheb(xs, i))
    i += 1
interact_manual(add_line);
```



In [6]:
```
def chebX(X, order):
    assert (-1 <= X).all() and (X <= 1).all()

    xs = []
    for c in range(order):
        xs.append(cheb(X, c))
    return t.cat(xs, 1)

N     = 10  # number of datapoints
D     = 1   # dimension of datapoints
sigma = 0.5 # output noise
t.manual_seed(0)
rand  = t.rand(N, 1)
X     = 2*rand - 1
Wtrue = t.tensor([[0.2], [0.5]])
Y     = chebX(X, 2) @ Wtrue + sigma*t.randn(N, 1)


def plot(order):
    Xe    = chebX(X, order)
    Wh    = fit_Wh(Xe, Y)
    print(f"Wtrue = {Wtrue.T}")
    print(f"Wh = {Wh.T}")

    fig, ax = plt.subplots()
    ax.set_xlabel("$x_\lambda$")
    ax.set_ylabel("$y_\lambda$")
    ax.set_xlim(-1, 1)
    ax.set_ylim(-2, 2)
    ax.scatter(X, Y, label="data");

    xs = t.linspace(-1, 1, 1000)[:, None]
    ax.plot(xs, chebX(xs, order)@Wh, 'r', label="fitted")
    ax.legend()

interact_manual(plot, order=IntSlider(min=1, max=10));
```

Cross-validation

How can we measure overfitting?

The standard approach is cross-validation, where we split the data into "training" and "validation" sets. We train the model on the training set, then look at the residuals/errors on the validation set.

The model with the smallest cross-validation error wins!

In [7]:
```
X_train = X[:7]
X_test = X[7:]

Y_train = Y[:7]
Y_test = Y[7:]

def plot(order):
    Wh    = fit_Wh(chebX(X_train, order), Y_train)

    Yh_test = chebX(X_test, order) @ Wh
    cross_validation_error = ((Y_test - Yh_test)**2).mean()
    print(f"cross validation error: {cross_validation_error}")

    fig, ax = plt.subplots()
    ax.set_xlabel("$x_\lambda$")
    ax.set_ylabel("$y_\lambda$")
    ax.set_xlim(-1, 1)
    ax.set_ylim(-2, 2)
    ax.scatter(X_train, Y_train, label="training data");
    ax.scatter(X_test, Y_test, label="validation data");
    ax.vlines(X_test, Y_test, Yh_test, label="test residuals")


    xs = t.linspace(-1, 1, 1000)[:, None]
    ax.plot(xs, chebX(xs, order)@Wh, 'r', label="fitted")
    ax.legend()

interact_manual(plot, order=IntSlider(min=1, max=10));
```

k-fold cross-validation

If you have relatively little data (as here), one thing you can do is to split your data up into train/validation sets in multiple different ways.

Regularisation

Cross-validation is great, but what if you've got lots of noise, and you can't control for that by just using a simple linear model?

Then, you don't want to give up on using the more complex basis functions to capture non-linearities.

Instead, we can penalise the weights, in particular,

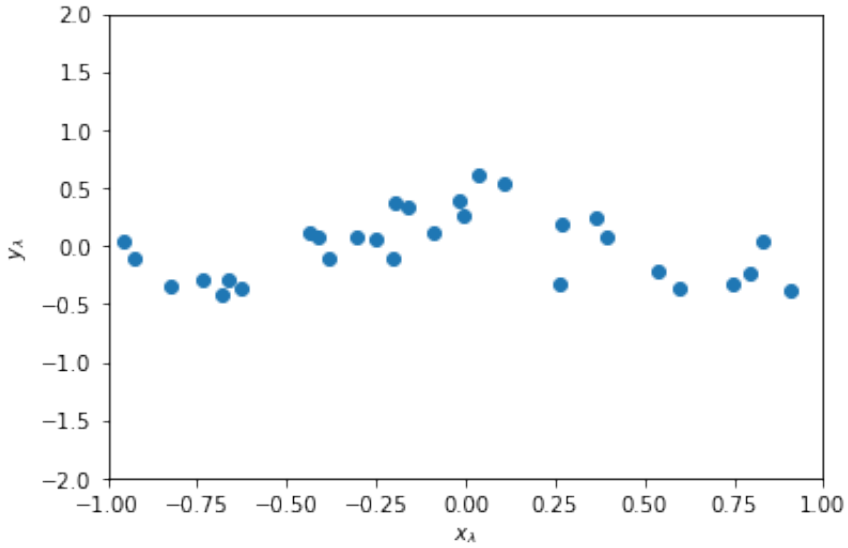
$$\mathcal{L}(\mathbf{w}) = \log \mathrm{P}\left(\mathbf{y}|\mathbf{X}, \mathbf{w}\right) - \tfrac{1}{2}\mathbf{w}^T\mathbf{\Lambda}\mathbf{w}$$

where we could (if we wanted) penalise different weights differently, using the diagonal matrix, $\mathbf{\Lambda}$.

As an exercise (in problem sheet), the solution of the corresponding optimization problem is,

$$\hat{\mathbf{W}} = \left(\left(\mathbf{X}^T\mathbf{X}\right)^{-1} + \sigma^2\mathbf{\Lambda}\right)^{-1}\mathbf{X}\mathbf{y}$$

In [8]:
```
N     = 30  # number of datapoints
D     = 1   # dimension of datapoints
sigma = 0.2 # output noise
t.manual_seed(0)
rand  = t.rand(N, 1)
X     = 2*rand - 1
Wtrue = t.tensor([[0.], [0.], [0.], [0.], [0.3]])
Y     = chebX(X, 5) @ Wtrue + sigma*t.randn(N, 1)

fig, ax = plt.subplots()
ax.set_xlabel("$x_\lambda$")
ax.set_ylabel("$y_\lambda$")
ax.set_xlim(-1, 1)
ax.set_ylim(-2, 2)

ax.scatter(X, Y);
```



In [9]:
```
X_train = X[:20]
X_test = X[20:]

Y_train = Y[:20]
Y_test = Y[20:]

def fit_reg_Wh(X, Y, reg):
    # reg = sigma**2 * Lambda
    return t.inverse(X.T @ X + reg*t.eye(X.shape[1])) @ X.T @ Y

def plot(order, reg):
    Wh    = fit_reg_Wh(chebX(X_train, order), Y_train, reg)

    Yh_test = chebX(X_test, order) @ Wh
    cross_validation_error = ((Y_test - Yh_test)**2).mean()
    print(f"cross validation error: {cross_validation_error}")
    print(f"Wh: {Wh.T}")

    fig, ax = plt.subplots()
    ax.set_xlabel("$x_\lambda$")
    ax.set_ylabel("$y_\lambda$")
    ax.set_xlim(-1, 1)
    ax.set_ylim(-2, 2)
    ax.scatter(X_train, Y_train, label="training data");
    ax.scatter(X_test, Y_test, label="validation data");
    ax.vlines(X_test, Y_test, Yh_test, label="test residuals")


    xs = t.linspace(-1, 1, 1000)[:, None]
    ax.plot(xs, chebX(xs, order)@Wh, 'r', label="fitted")
    ax.legend()

interact_manual(plot, order=IntSlider(min=1, max=12), reg=FloatSlid
er(min=0, max=2));
```

Note that in this example, the corollary of overfitting is the estimated weights getting really big.

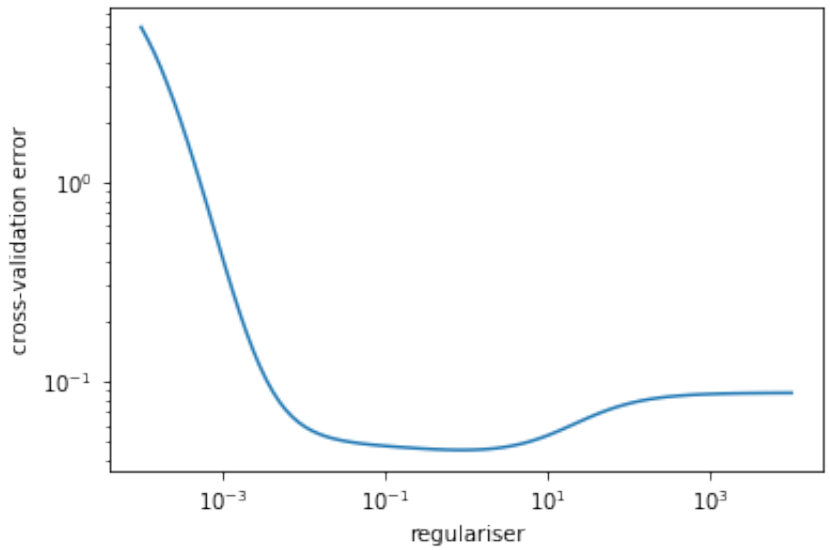
Regularisation explicitly penalises large weights, and gives more sensible solutions.

Automatic selection of the regulariser using cross-validation

Now things are even worse. Before, we just had to choose the "function complexity", which was a smallish integer. Now we have to choose a regulariser, and we don't even know what type of size the regulariser should be.

The only thing we can do is to use cross-validation!

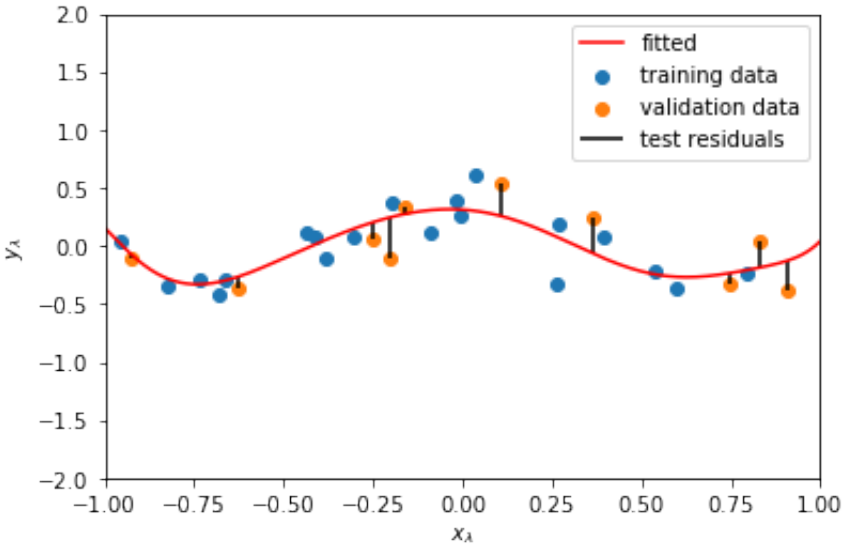
In [10]:
```
def cv(order, reg):
    Wh    = fit_reg_Wh(chebX(X_train, order), Y_train, reg)

    Yh_test = chebX(X_test, order) @ Wh
    return ((Y_test - Yh_test)**2).mean()

log_10_regs = np.linspace(-4, 4, 100)
regs = 10**log_10_regs
cv_errors = np.array([cv(10, reg) for reg in regs])

fig, ax = plt.subplots()
ax.set_xlabel("regulariser")
ax.set_ylabel("cross-validation error")
ax.set_xscale('log')
ax.set_yscale('log')
ax.plot(regs, cv_errors);
```



Now we can select the regulariser with the lowest cross-validation error.

In [11]:
```
best_reg = regs[np.argmin(cv_errors)]
plot(order=10, reg=best_reg)
```

```
cross validation error: 0.04509706050157547
Wh: tensor([[-0.0478, -0.0224, -0.0798,  0.0029,  0.2467, -0.0567,
-0.0267,  0.0039,
          0.0076,  0.0156]])
```



Limits of cross-validation

There's a bunch of issues with cross-validation:

- Parameter sweeps can be numerically costly.
- Splitting your data gives you less data for training, which is very problematic with smaller amounts of data.
- Scales poorly if you want to cross-validate many different parameters.