PyTorch main functionalities

1. Automatic gradient calculations

2. GPU acceleration (probably won't cover in class)

3. Neural network functions (simplify things a good deal)

(PyTorch has a very nice tutorial that covers more basics: [https://pytorch.org/tutorials/beginner/basics/intro.html (https://pytorch.org/tutorials/beginner/basics/intro.html)](https://pytorch.org/tutorials/beginner/basics/intro.html))

In [1]:

```python
import numpy as np
import torch # PyTorch library
import scipy.stats
import matplotlib.pyplot as plt
import seaborn as sns
# To visualize computation graphs
# See: https://github.com/szagoruyko/pytorchviz
# Uncomment the following line to install on Google colab
#%pip install -U git+https://github.com/szagoruyko/pytorchviz.git@master
from torchviz import make_dot, make_dot_from_trace
sns.set()
%matplotlib inline
```

PyTorch: Some basics of converting between NumPy and Torch

See link below for more information: [https://pytorch.org/tutorials/beginner/former_torchies/tensor_tutorial.html#numpy-bridge (https://pytorch.org/tutorials/beginner/former_torchies/tensor_tutorial.html#numpy-bridge)](https://pytorch.org/tutorials/beginner/former_torchies/tensor_tutorial.html#numpy-bridge)

In [2]:

```
# Torch and numpy
x = torch.linspace(-5,5,10)
print(x)
print(x.dtype)
print('NOTE: x is float32 (torch default is float32)')
x_np = np.linspace(-5,5,10)
y = torch.from_numpy(x_np)
print(y)
print(y.dtype)
print('NOTE: y is float64 (numpy default is float64)')
print(y.float().dtype)
print('NOTE: y can be converted to float32 via `float()`')
print(x.numpy())
print(y.numpy())
```

```
tensor([-5.0000, -3.8889, -2.7778, -1.6667, -0.5556,  0.5556,  1.6667,
2.7778,
         3.8889,  5.0000])
torch.float32
NOTE: x is float32 (torch default is float32)
tensor([-5.0000, -3.8889, -2.7778, -1.6667, -0.5556,  0.5556,  1.6667,
2.7778,
         3.8889,  5.0000], dtype=torch.float64)
torch.float64
NOTE: y is float64 (numpy default is float64)
torch.float32
NOTE: y can be converted to float32 via `float()`
[-5.         -3.8888888  -2.7777777  -1.6666665  -0.55555534  0.55555534
  1.6666665   2.7777777   3.8888888   5.        ]
[-5.         -3.88888889 -2.77777778 -1.66666667 -0.55555556  0.55555556
  1.66666667  2.77777778  3.88888889  5.        ]
```

Torch can be used to do simple computations just like numpy

In [3]:

```
# Explore gradient calculations
x = torch.tensor(5.0)
y = 3*x**2 + x
print(x, x.grad)
print(y)
```

```
tensor(5.) None
tensor(80.)
```

PyTorch automatically creates a computation graph for computing gradients if `requires_grad=True`

IMPORTANT: You must set `requires_grad=True` for any torch tensor for which you will want to compute the gradient (usually model parameters)

These are known as the "leaf nodes" or "input nodes" of a gradient computation graph

Note that some leaf nodes will not need gradient (e.g., constant matrices like the training data)

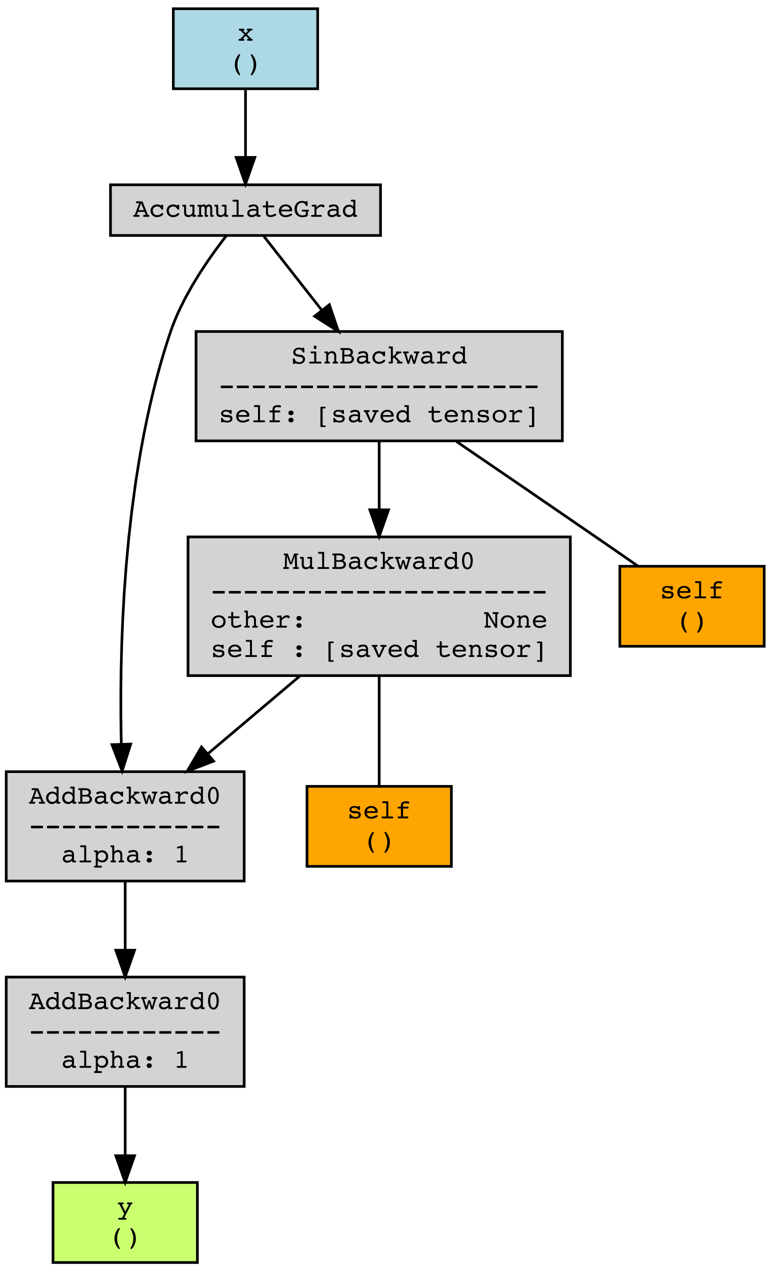
Okay let's compute and show the computation graph

In [4]:

```python
# Explore gradient calculations
x = torch.tensor(5.0, requires_grad=True)
c = torch.tensor(3.0)  # A constant input tensor that does not require grad
#y = c*x**2 + x+c
y = c*torch.sin(x) + x + c
print(x, x.grad)
print(y)
make_dot(y, dict(x=x, c=c, y=y), show_attrs=True, show_saved=True)
```

```
tensor(5., requires_grad=True) None
tensor(5.1232, grad_fn=<AddBackward0>)
```

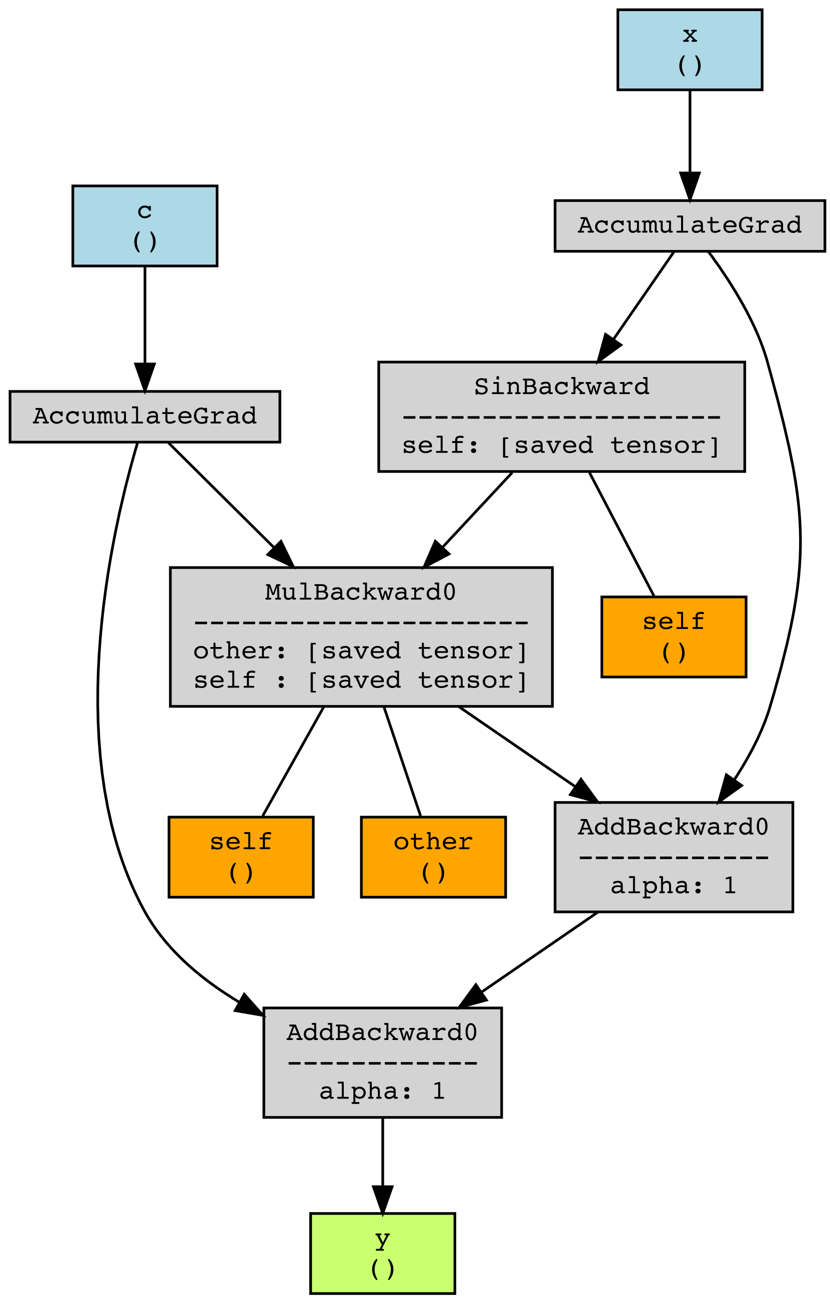
Out[4]:



In [5]:
```
# Explore gradient calculations
x = torch.tensor(5.0, requires_grad=True)
c = torch.tensor(3.0, requires_grad=True)  # Change to compute grad over th
#y = c*x**2 + x+c
y = c*torch.sin(x) + x + c
print(x, x.grad)
print(y)
make_dot(y, dict(x=x, c=c, y=y), show_attrs=True, show_saved=True)
```

```
tensor(5., requires_grad=True) None
tensor(5.1232, grad_fn=<AddBackward0>)
```

Out[5]:

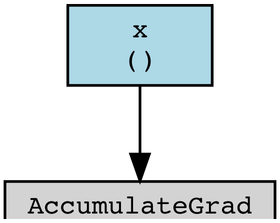


In [6]:

```
# We can even do loops
x = torch.tensor(1.0, requires_grad=True)
y = x
for i in range(3):
    y = y*(y+1)
print(x, x.grad)
print(y)
make_dot(y, dict(x=x, y=y), show_attrs=True, show_saved=True)
```

```
tensor(1., requires_grad=True) None
tensor(42., grad_fn=<MulBackward0>)
```

Out[6]:



Let's do this for a more complex ML example

Below is a simple linear regression error computation for a random model

In [7]:

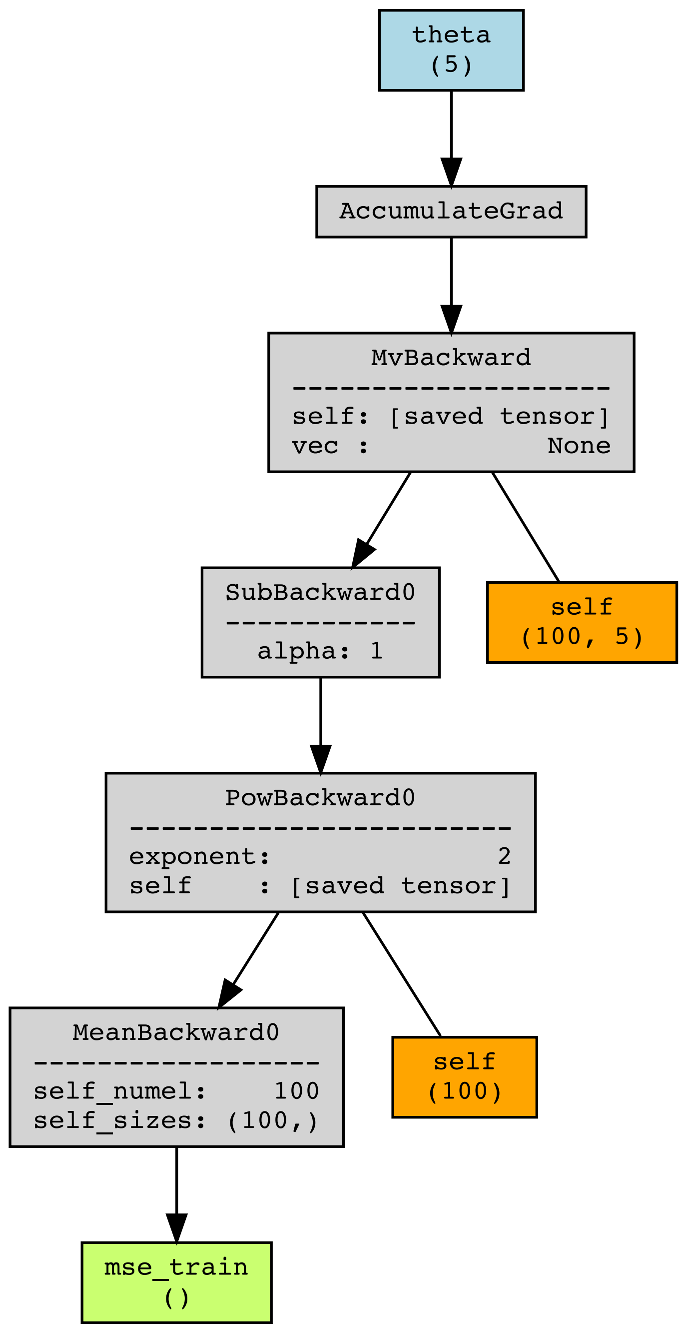
```python
# A simple tensor example
# Data
rng = torch.manual_seed(42)
X_train = torch.randn(100, 5) #.requires_grad_(True)
y_train = torch.mean(X_train, axis=1)  # Average of x features

# Model
theta = torch.randn(5).requires_grad_(True)
y_pred = torch.matmul(X_train, theta)

# Error
mse_train = torch.mean((y_train - y_pred)**2)

make_dot(mse_train, dict(X_train=X_train, mse_train=mse_train, theta=theta))
```

Out[7]:



While only the parameters should "require_grad" in usual ML optimization, you could compute gradients for other inputs (e.g., creating adversarial examples via optimization)

In [8]:

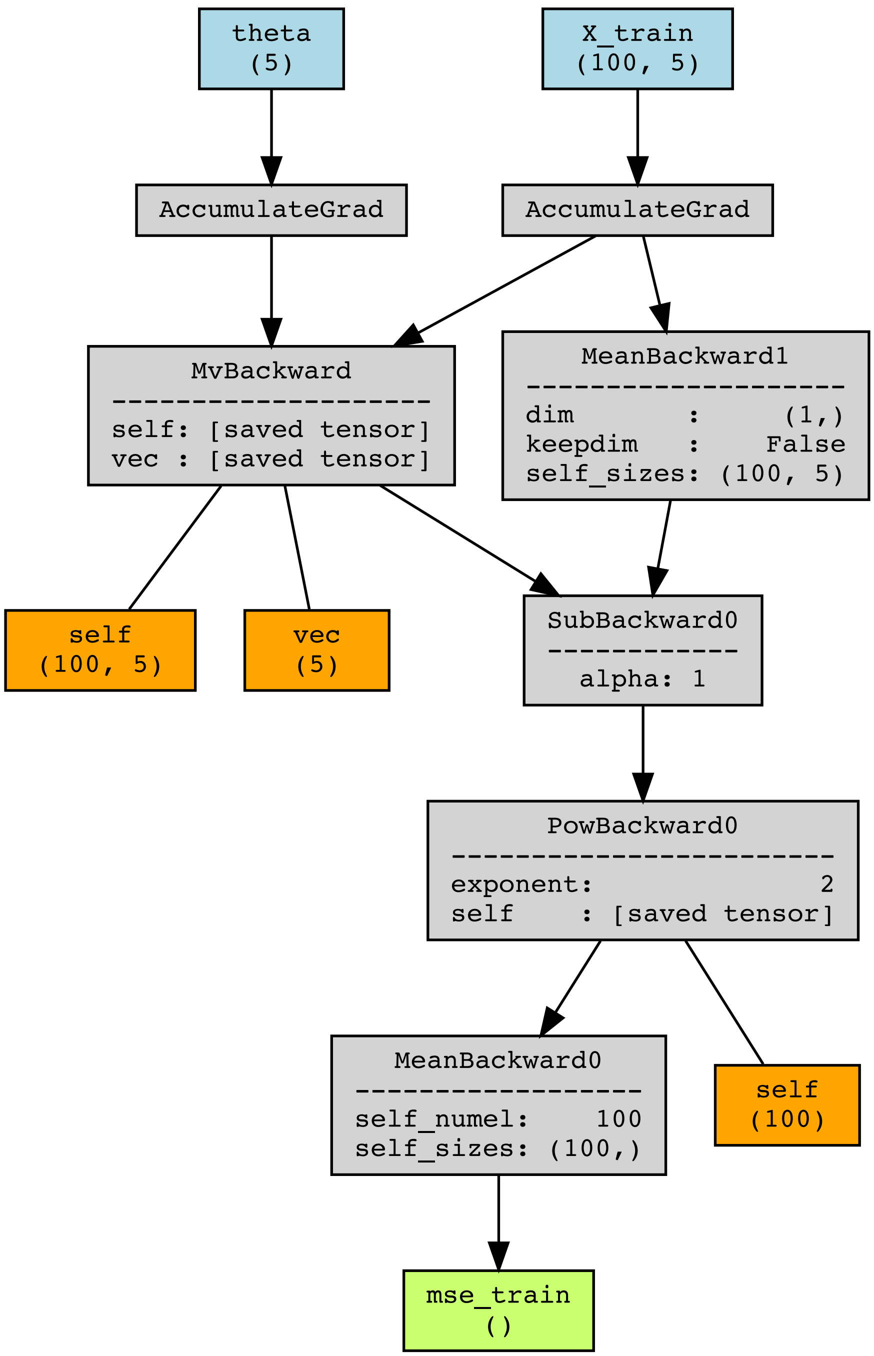
```
# A simple tensor example
# Data
rng = torch.manual_seed(42)
X_train = torch.randn(100, 5).requires_grad_(True)
y_train = torch.mean(X_train, axis=1)  # Average of x features

# Model
theta = torch.randn(5).requires_grad_(True)
y_pred = torch.matmul(X_train, theta)

# Error
mse_train = torch.mean((y_train - y_pred)**2)

make_dot(mse_train, dict(X_train=X_train, mse_train=mse_train, theta=theta))
```

Out[8]:



Now we can automatically compute gradients via backward call

Note that tensor has grad_fn for doing the backwards computation

In [9]:
```
x = torch.tensor(5.0, requires_grad=True)
c = torch.tensor(3.0)  # A constant input tensor that does not require grad
#y = c*x**2 + x+c
y = c*torch.sin(x) + x + c
print(x, x.grad)
print(y)

y.backward()
print(x, x.grad)
print(y)
```

```
tensor(5., requires_grad=True) None
tensor(5.1232, grad_fn=<AddBackward0>)
tensor(5., requires_grad=True) tensor(1.8510)
tensor(5.1232, grad_fn=<AddBackward0>)
```

A call to `backward` will free up the implicit computation graph (i.e., removed saved tensors)

In [10]:
```
try:
    y.backward()
    print(x, x.grad)
    print(y)
except Exception as e:
    print(e)
```

```
Trying to backward through the graph a second time (or directly access sa
ved variables after they have already been freed). Saved intermediate val
ues of the graph are freed when you call .backward() or autograd.grad().
Specify retain_graph=True if you need to backward through the graph a sec
ond time or if you need to access saved variables after calling backward.
```

Gradients accumulate, i.e., sum, from multiple backward calls

```
In [11]: x = torch.tensor(5.0, requires_grad=True)
for i in range(2):
    y = 3*x**2
    y.backward()
    print(x, x.grad)
    print(y)
```

```
tensor(5., requires_grad=True) tensor(30.)
tensor(75., grad_fn=<MulBackward0>)
tensor(5., requires_grad=True) tensor(60.)
tensor(75., grad_fn=<MulBackward0>)
```

Thus, must zero gradients before calling `backward()`

```
In [12]: # Thus if before calling another gradient iteration, zero the gradients
x.grad.zero_()
print(x, x.grad)

# Now that gradient is zero, we can do again
y = 3*x**2
y.backward()
print(x, x.grad)
print(y)
```

```
tensor(5., requires_grad=True) tensor(0.)
tensor(5., requires_grad=True) tensor(30.)
tensor(75., grad_fn=<MulBackward0>)
```

More complicated gradients example

```
In [13]: x = torch.arange(5, dtype=torch.float32).requires_grad_(True)
y = torch.mean(torch.log(x**2+1)+5*x)
y.backward()
print(y)
print(x)
print('Grad', x.grad)
```

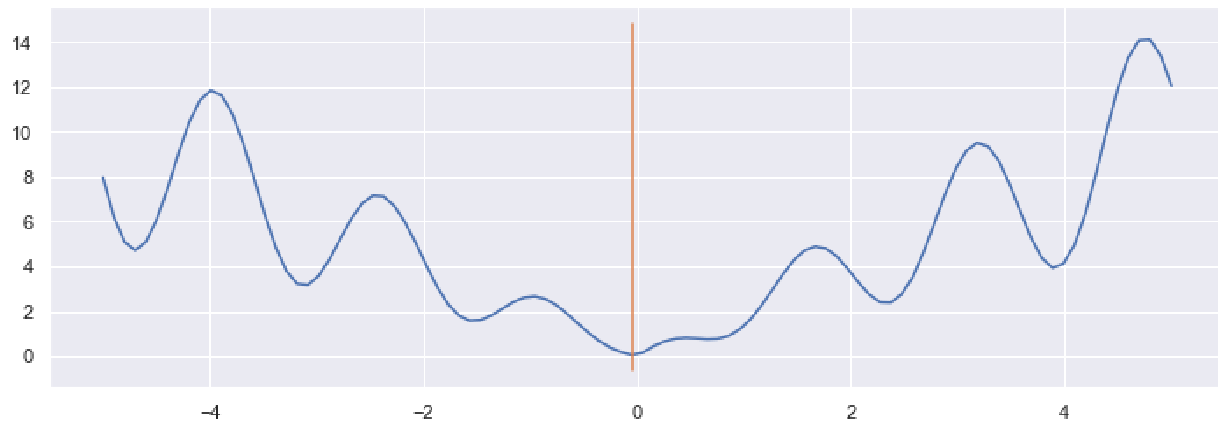
```
tensor(11.4877, grad_fn=<MeanBackward0>)
tensor([0., 1., 2., 3., 4.], requires_grad=True)
Grad tensor([1.0000, 1.2000, 1.1600, 1.1200, 1.0941])
```

Now let's optimize a non-convex function (pretty much all DNNs)

In [14]:
```
def objective(theta):
    return theta*torch.cos(4*theta) + 2*torch.abs(theta)

theta = torch.linspace(-5, 5, steps=100)
y = objective(theta)
theta_true = float(theta[np.argmin(y)])
plt.figure(figsize=(12,4))
plt.plot(theta.numpy(), y.numpy())
plt.plot(theta_true * np.ones(2), plt.ylim())
```

Out[14]:
```
[<matplotlib.lines.Line2D at 0x7fab91014100>]
```



Let's use simple gradient descent on this function

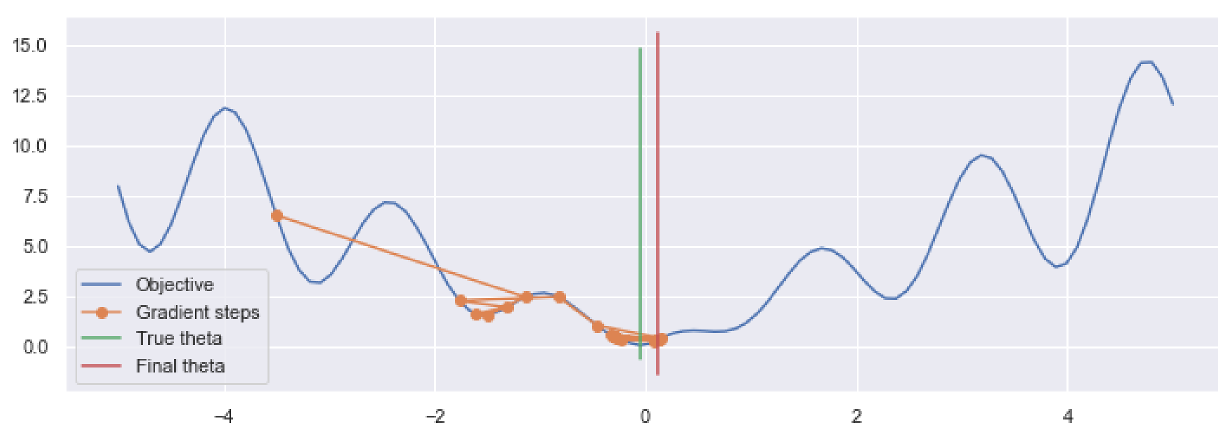
In [15]:
```
def gradient_descent(objective, step_size=0.05, max_iter=100, init=0):
    # Initialize
    theta_hat = torch.tensor(init, requires_grad=True)
    theta_hat_arr = [theta_hat.detach().numpy().copy()]
    obj_arr = [objective(theta_hat).detach().numpy()]
    # Iterate
    for i in range(max_iter):
        # Compute gradient
        if theta_hat.grad is not None:
            theta_hat.grad.zero_()
        out = objective(theta_hat)
        out.backward()

        # Update theta in-place
        with torch.no_grad():
            theta_hat -= step_size * theta_hat.grad
        theta_hat_arr.append(theta_hat.detach().numpy().copy())
        obj_arr.append(objective(theta_hat).detach().numpy())
    return np.array(theta_hat_arr), np.array(obj_arr)

def visualize_results(theta_arr, obj_arr, objective, theta_true=None, vis_a
    if vis_arr is None:
        vis_arr = np.linspace(np.min(theta_arr), np.max(theta_arr))
    fig = plt.figure(figsize=(12,4))
    plt.plot(vis_arr, [objective(torch.tensor(theta)).numpy() for theta in
    plt.plot(theta_arr, obj_arr, 'o-', label='Gradient steps')
    if theta_true is not None:
        plt.plot(np.ones(2)*theta_true, plt.ylim(), label='True theta')
    plt.plot(np.ones(2)*theta_arr[-1], plt.ylim(), label='Final theta')
    plt.legend()

# 0.05 doesn't escape, 0.07 does, 0.15 gets much closer
theta_hat_arr, obj_arr = gradient_descent(
    objective, step_size=0.15, init=-3.5, max_iter=100)

visualize_results(theta_hat_arr, obj_arr, objective, theta_true=theta_true,
```



Putting it all together for ML models

PyTorch has many helper functions to handle much of stochastic gradient descent or using other optimizers

Example from
https://pytorch.org/tutorials/beginner/examples_nn/two_laye
(https://pytorch.org/tutorials/beginner/examples_nn/two_lay

In [16]:
```python
import torch

# N is batch size; D_in is input dimension;
# H is hidden dimension; D_out is output dimension.
N, D_in, H, D_out = 64, 1000, 100, 10

# Create random Tensors to hold inputs and outputs
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)

# Use the nn package to define our model and loss function.
model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out),
)
loss_fn = torch.nn.MSELoss(reduction='sum')

# Use the optim package to define an Optimizer that will update the weights
# the model for us. Here we will use Adam; the optim package contains many
# optimization algoriths. The first argument to the Adam constructor tells
# optimizer which Tensors it should update.
learning_rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
for t in range(500):
    # Forward pass: compute predicted y by passing x to the model.
    y_pred = model(x)

    # Compute and print loss.
    loss = loss_fn(y_pred, y)
    if t % 100 == 99:
        print(t, loss.item())

    # Before the backward pass, use the optimizer object to zero all of the
    # gradients for the variables it will update (which are the learnable
    # weights of the model). This is because by default, gradients are
    # accumulated in buffers( i.e, not overwritten) whenever .backward()
    # is called. Checkout docs of torch.autograd.backward for more details.
    optimizer.zero_grad()

    # Backward pass: compute gradient of the loss with respect to model
    # parameters
    loss.backward()

    # Calling the step function on an Optimizer makes an update to its
    # parameters
    optimizer.step()
```

```
99 71.03111267089844
199 1.6399927139282227
299 0.015610104426741 6
399 6.423537706723437e-05
499 8.300153808704636e-08
```

A few more details `autograd` and `backward()`

function

See https://pytorch.org/tutorials/beginner/basics/autogradqs_tutorial.html (https://pytorch.org/tutorials/beginner/basics/autogradqs_tutorial.html) for more details.

Jacobian

$$J = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

Backward computes Jacobian transpose vector product

$$J^T \cdot v = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix} \begin{pmatrix} \frac{\partial l}{\partial y_1} \\ \vdots \\ \frac{\partial l}{\partial y_m} \end{pmatrix} = \begin{pmatrix} \frac{\partial l}{\partial x_1} \\ \vdots \\ \frac{\partial l}{\partial x_n} \end{pmatrix}$$

Simplification is when output is scalar than the derivative is assumed to be 1

Example: $y = b^T x, z = \exp(y)$

- $J_z = [[\frac{dz}{dy}]], v = [1], J_z^T v = \frac{dz}{dy}$
- $J_y = \left[\frac{dy}{dx_1} \quad \frac{dy}{dx_2} \quad \cdots \quad \frac{dy}{dx_5} \right]^T, v = \frac{dz}{dy}, J_y^T v = \left[\frac{dz}{dx_1} \quad \frac{dz}{dx_2} \quad \cdots \quad \frac{dz}{dx_5} \right]^T = \nabla_x z(x)$

In [17]:
```
x = (2.0 * torch.ones(5).float()).requires_grad_(True)
b = torch.arange(5).float()
y = torch.dot(b, x)
y.retain_grad()
z = torch.log(y)
z.retain_grad()
z.backward()

def print_grad(a):
    print(a, a.grad)
print_grad(z)
print_grad(y)
print_grad(x)
```

```
tensor(2.9957, grad_fn=<LogBackward>) tensor(1.)
tensor(20., grad_fn=<DotBackward>) tensor(0.0500)
tensor([2., 2., 2., 2., 2.], requires_grad=True) tensor([0.0000, 0.0500,
0.1000, 0.1500, 0.2000])
```