Optimization

- In Deep Learning, we *train* models, updating them successively so that they get better and better as they see more and more training data.
    - *Optimization*: the process of fitting our models to observed data
    - To understand optimization problems and methods, we need to know basic concepts from *Calculus*.

Recap from last week

- Estimate blood pressure from height, weight, age, exerc_hours

In [1]:
```
%matplotlib inline

# input_data X: [height, weight, age, exerc_hours]
X = [[180, 89, 35, 1],
     [160, 49, 40, 4],
     [179, 69, 20, 2]];

# ground truth values Y: blood_pressure
Y = [[160], [130], [110]];
```

- If the model parameters are known:

In [2]:
```
# model w: w = [w0, w1, w2, w3]
w = [0.3, 0.8, -0.4, 10];

def model(w, x):
    y_hat = w[0]*x[0]+w[1]*x[1]+w[2]*x[2]+w[3]*x[3]
    return y_hat

x0 = X[0]
y0_hat = model(w, x0)
print(y0_hat)
```

```
121.2
```

- If the model parameters are *unknown*, we can use ground truth labels to find them

$$loss = (y - \hat{y})^2$$

In [3]:
```
def loss(y, y_hat):
    return (y-y_hat)**2

y0 = Y[0][0]
print(loss(y0, y0_hat))
```

```
1505.4399999999998
```

- The update for the first parameter $w[0]$ is given by:

$$w[0] \leftarrow w[0] - \frac{\theta loss}{\theta w[0]}$$

- In this lecture, we will see what $\frac{\theta loss}{\theta w[0]}$ is all about.
- For that, we need to know basic concepts from *Calculus*.

Functions

- In maths, functions are similar to functions in programming
- Given a set of input values, a function can be used to compute an output

In [4]:
```python
# Python:
def f(w, x):
    y = w[0]*x[0]+w[1]*x[1]+w[2]*x[2]+w[3]*x[3]
    return y
```

- Maths:

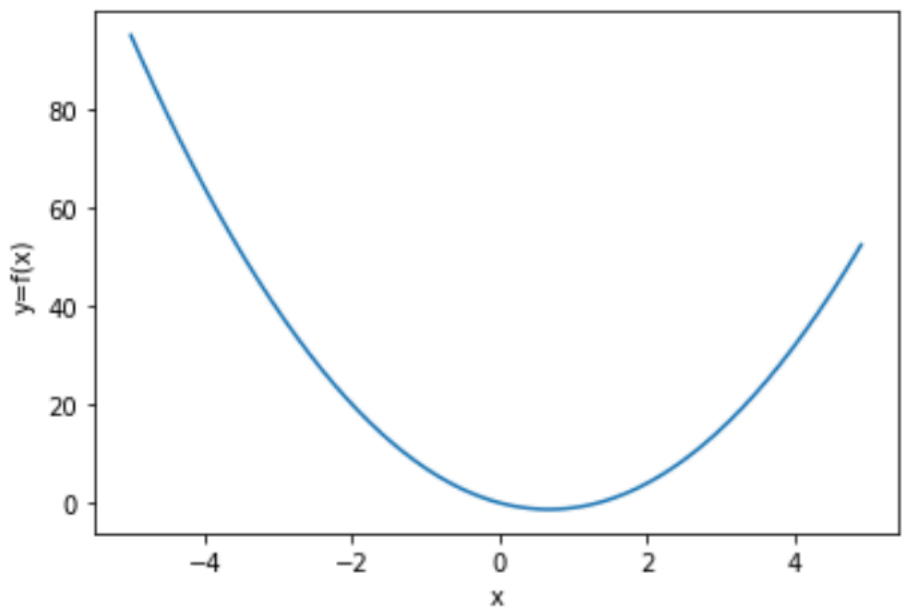
$$y = f(w_0, w_1, w_2, w_3, x_0, x_1, x_2, x_3)$$

$$y = w_0 \cdot x_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + w_3 \cdot x_3$$

- The above function has 8 input variables.
- Let's assume for simplicity a single variable function: $y = f(x)$ where $f : \mathbb{R} \to \mathbb{R}$.
- Example: Define the function $f(x) = 3x^2 - 4x$.

In [1]:

```
import torch
from matplotlib import pyplot as plt
%matplotlib inline

def f(x):
    return 3 * x ** 2 - 4 * x

x = torch.arange(-5, 5, 0.1)
y = f(x)
plt.plot(x,y);
plt.xlabel('x'); plt.ylabel('y=f(x)');
```



Derivatives and Differentiation

- Suppose that we have a function $f : \mathbb{R} \to \mathbb{R}$, whose input and output are both scalars. The *derivative* of f is defined as:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h},$$

  if this limit exists.

- We can interpret the derivative $f'(x)$ as the *instantaneous* rate of change of $f(x)$ with respect to x.

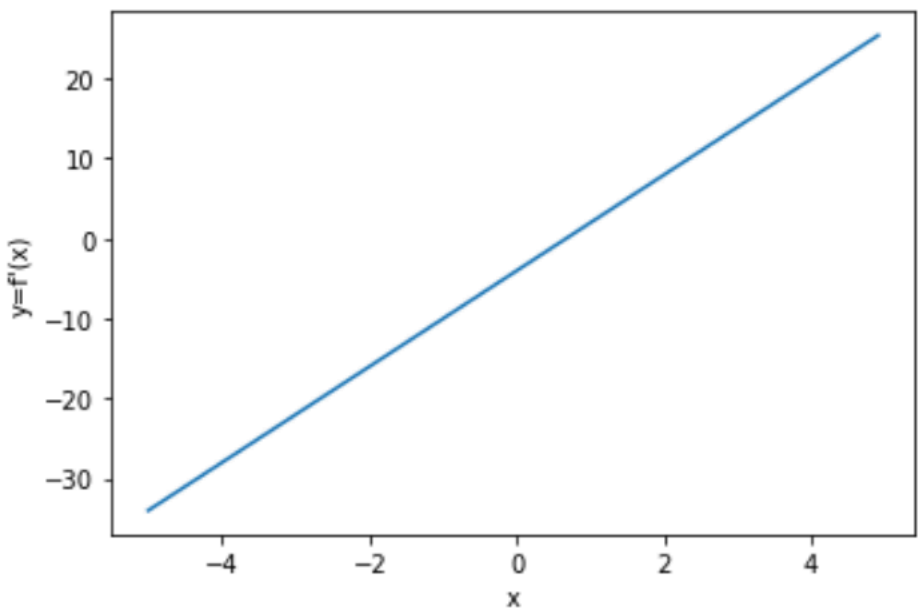
- Example: Consider again the function $f(x) = 3x^2 - 4x$. For $x = 1$ and by letting h approach 0, the derivative $f'(x)$ is getting equal to 2.

In [6]:
```
%matplotlib inline

def f(x):
    return 3 * x ** 2 - 4 * x

def numerical_lim(f, x, h):
    return (f(x + h) - f(x)) / h

h = 0.1
for i in range(5):
    print(f'h={h:.5f}, numerical limit={numerical_lim(f, 1, h):.5f}')
    h *= 0.1
```

```
h=0.10000, numerical limit=2.30000
h=0.01000, numerical limit=2.03000
h=0.00100, numerical limit=2.00300
h=0.00010, numerical limit=2.00030
h=0.00001, numerical limit=2.00003
```

- If f is differentiable at every number of an interval, then this function is differentiable on this interval.
- This also means that the derivative is also a function.
- For example the derivative of $f(x) = 3x^2 - 4x$ is also function $f'(x) = 6x - 4$.

In [4]:
```
def f_prime(x):
    return 6 * x - 4

x = torch.arange(-5, 5, 0.1)
plt.plot(x,f_prime(x));
plt.xlabel('x'); plt.ylabel("y=f'(x)");
```



Differentiation rules

- Given $y = f(x)$, the following expressions are equivalent:

$$f'(x) = y' = \frac{dy}{dx} = \frac{df}{dx} = \frac{d}{dx} f(x) = Df(x) = D_x f(x),$$

where symbols $\frac{d}{dx}$ and D are *differentiation operators* that indicate operation of *differentiation*.

- Differentiation results of commonly-used functions:
  - $DC = 0$ (C is a constant),
  - $Dx^n = nx^{n-1}$ (the *power rule*, n is any real number),
  - $De^x = e^x$,
  - $D \ln(x) = 1/x$.
- The above results are just examples: there are many more functions for which the derivatives are readily available.

- Suppose that functions f and g are both differentiable and C is a constant, we have:
  - the *constant multiple rule*

$$\frac{d}{dx}[Cf(x)] = C\frac{d}{dx}f(x),$$

  - the *sum rule*

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx}f(x) + \frac{d}{dx}g(x),$$

  - the *product rule*

$$\frac{d}{dx}[f(x)g(x)] = f(x)\frac{d}{dx}[g(x)] + g(x)\frac{d}{dx}[f(x)],$$

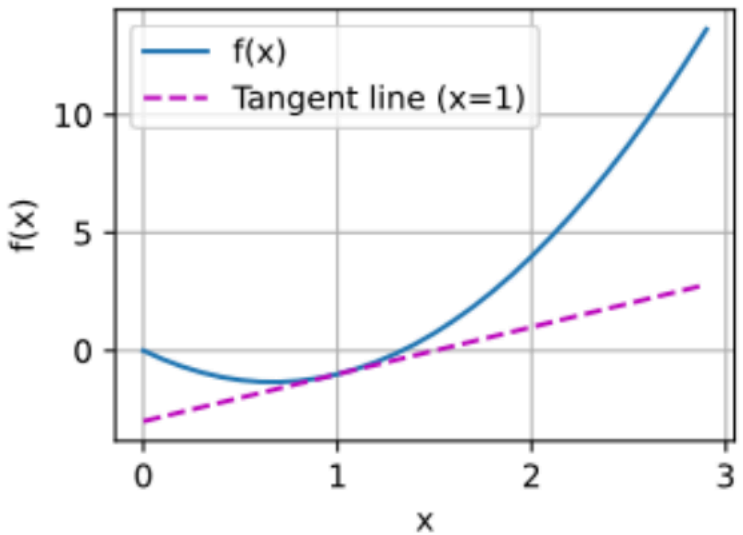
  - and the *quotient rule*

$$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)\frac{d}{dx}[f(x)] - f(x)\frac{d}{dx}[g(x)]}{[g(x)]^2}.$$

- Now we can apply a few of the above rules to find $f'(x) = 3\frac{d}{dx}x^2 - 4\frac{d}{dx}x = 6x - 4$. Thus, by setting $x = 1$, we have $f'(1) = 2$.

Visualization

- This derivative is also the slope of the tangent line to the curve $f(x)$ when $x = 1$.



Partial Derivatives

- So far we have dealt with the differentiation of functions of just one variable.
- In deep learning, functions often depend on *many* variables. Thus, we need to extend the ideas of differentiation to these *multivariate* functions.
- Let $y = f(x_1, x_2, \ldots, x_n)$ be a function with n variables.
- Function f takes the n variables $x_1, x_2, \ldots, x_n$ and maps them to a single number, i.e. y is *scalar*.
- Equivalently, we can write $y = f(\mathbf{x})$ where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top$ is the n-dimensional vector containing the input variables.
- Example from above:

$$y = w_0 \cdot x_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + w_3 \cdot x_3$$

- The *partial derivative* of y with respect to its i^{th} parameter x_i is:
$$\frac{\partial y}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, \ldots, x_{i-1}, x_i + h, x_{i+1}, \ldots, x_n) - f(x_1, \ldots, x_i, \ldots, x_n)}{h}.$$

- To calculate $\frac{\partial y}{\partial x_i}$, we can simply treat $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n$ as constants and calculate the derivative of y with respect to x_i.

- In terms of notation of partial derivatives, the following are equivalent:
$$\frac{\partial y}{\partial x_i} = \frac{\partial f}{\partial x_i} = f_{x_i} = f_i = D_i f = D_{x_i} f.$$

Gradients

- We can concatenate partial derivatives of a multivariate function $f(\mathbf{x})$ with respect to all its input variables to obtain the *gradient* vector of the function.
- The gradient of the function $f(\mathbf{x})$ with respect to $\mathbf{x}$ is a vector of n partial derivatives:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \cdots, \frac{\partial f(\mathbf{x})}{\partial x_n}\right]^\top,$$

where $\nabla_{\mathbf{x}} f(\mathbf{x})$ is often replaced by $\nabla f(\mathbf{x})$ when there is no ambiguity.

Differentiation results of commonly-used multivariate functions

The following results are often used when differentiating multivariate functions:

- $\nabla_{\mathbf{x}} \mathbf{A}\mathbf{x} = \mathbf{A}^\top$
- $\nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A} = \mathbf{A}$
- $\nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A}\mathbf{x} = (\mathbf{A} + \mathbf{A}^\top)\mathbf{x}$
- $\nabla_{\mathbf{x}} \|\mathbf{x}\|^2 = \nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{x} = 2\mathbf{x}$

Chain Rule

- In Deep Learning, the multivariate functions used are often *composite*, so the above rules cannot be directly applied.
- Fortunately, the *chain rule* enables the differentiatiation of composite functions.
- Let us first consider functions of a single variable. Suppose that functions $y = f(u)$ and $u = g(x)$ are both differentiable, then the chain rule states that

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}.$$

- Suppose now that the differentiable function y has variables $u_1, u_2, \ldots, u_m$, where each differentiable function u_i has variables $x_1, x_2, \ldots, x_n$. Note that y is a function of $x_1, x_2, \ldots, x_n$.
- Then, the chain rule gives

$$\frac{dy}{dx_i} = \frac{dy}{du_1}\frac{du_1}{dx_i} + \frac{dy}{du_2}\frac{du_2}{dx_i} + \cdots + \frac{dy}{du_m}\frac{du_m}{dx_i}$$

for any $i = 1, 2, \ldots, n$.

Automatic Differentiation

- Differentiation is a crucial step in nearly all deep learning optimization algorithms.
- While the calculations for taking these derivatives is doable, for complex models, working out the calculations by hand can be a pain (and often error-prone).
- Deep learning frameworks overcome this problem by automatically calculating derivatives, by *automatic differentiation*.
- Given a model the system builds a *computational graph*, tracking which data combined through which operations to produce the output.
- Automatic differentiation enables the system to subsequently calculate gradients.

A Simple Example

- Differentiate function $y = 2\mathbf{x}^\top \mathbf{x}$ with respect to the column vector $\mathbf{x}$.
- Note that, in practice, AD allows the calculation of the derivative for a specific value of the input variable.
- It does not provide a general mathematical formula for the function derivative.
    - Good news is that you never need the formula in practice.
- For example consider the function $f(x) = 3x^2 - 4x$. We know that its derivative is $f'(x) = 6x - 4$. AD will not give you access to this formula. It will give you access to values of $f'(x)$ for specific input values of x, e.g. $f'(1) = f'(x)$ for $x = 1$, $f'(10) = f'(x)$ for $x = 10$ etc.

In [2]:

```
import torch
# create a specific value of input x
x = torch.arange(4.0)
x.requires_grad_(True)
print(x)
print(x.grad)
y = 2*torch.dot(x, x)
print(y)
```

```
tensor([0., 1., 2., 3.], requires_grad=True)
None
tensor(28., grad_fn=<MulBackward0>)
```

- Next, we can automatically calculate the gradient of `y` with respect to each component of `x` by calling the function for gradient calculation and printing the gradient.
- This function is called **backpropagation**

In [3]:
```
y.backward()
x.grad
```

Out[3]:
```
tensor([ 0.,  4.,  8., 12.])
```

- The gradient of the function $y = 2\mathbf{x}^\top \mathbf{x}$ with respect to $\mathbf{x}$ should be $4\mathbf{x}$.
- Let us quickly verify that our desired gradient was calculated correctly.

In [4]:
```
x.grad == 4 * x
```

Out[4]:
```
tensor([True, True, True, True])
```

In [5]:
```
# Another example y = h(x) = x1+x2+x3+x4
# PyTorch accumulates the gradient in default, we need to clear the previous
# values
x.grad.zero_()
y = x.sum()
y.backward()
x.grad
```

Out[5]:
```
tensor([1., 1., 1., 1.])
```

In [6]:
```
# output y must be always scalar
x.grad.zero_()
y = x * x
y.backward() # will throw an error
x.grad
```

```
---------------------------------------------------------------------------
RuntimeError                              Traceback (most recent call last)
<ipython-input-6-109fe2573949> in <module>()
      2 x.grad.zero_()
      3 y = x * x
----> 4 y.backward() # will throw an error
      5 x.grad

/usr/local/lib/python3.6/dist-packages/torch/tensor.py in backward(self, gradi
ent, retain_graph, create_graph)
    219                 retain_graph=retain_graph,
    220                 create_graph=create_graph)
--> 221         torch.autograd.backward(self, gradient, retain_graph, create_g
raph)
    222
    223     def register_hook(self, hook):

/usr/local/lib/python3.6/dist-packages/torch/autograd/__init__.py in backward
(tensors, grad_tensors, retain_graph, create_graph, grad_variables)
    124
    125     grad_tensors_ = _tensor_or_tensors_to_tuple(grad_tensors, len(tens
ors))
--> 126     grad_tensors_ = _make_grads(tensors, grad_tensors_)
    127     if retain_graph is None:
    128         retain_graph = create_graph

/usr/local/lib/python3.6/dist-packages/torch/autograd/__init__.py in _make_gra
ds(outputs, grads)
     48             if out.requires_grad:
```

Detaching Computation

- Sometimes, we wish to move some calculations outside of the recorded computational graph.
- Example: consider $f(x) = 2\mathbf{x}^\top \mathbf{x}$ and then function $g(x) = (f(x) - \alpha)^2$ where α is a constant. Let's asssume $\alpha = 2$.

In [7]:
```
# create a specific value of input x
x = torch.arange(4.0)
x.requires_grad_(True)
f = 2*torch.dot(x, x)
a = 2
g = (f-a)**2
g.backward()
print(x.grad)
```

```
tensor([  0., 208., 416., 624.])
```

- Now consider the case where $\alpha = x_1 + x_2 + x_3 + x_4$
- If we want α to be treated as constant i.e. $\alpha = 0 + 1 + 2 + 3 = 6$ then we must *detach* α from the graph!
- Otherwise it will be considered a function of input $\mathbf{x}$!

In [8]:
```
x = torch.arange(4.0)
x.requires_grad_(True)
f = 2*torch.dot(x, x)
a = x.sum().detach() #equivalent to a = 6
#a = x.sum() # here a is a function of x
g = (f-a)**2
g.backward()
print(x.grad)
```

```
tensor([  0., 176., 352., 528.])
```

In [9]:

```
x = torch.arange(4.0)
x.requires_grad_(True)
f = 2*torch.dot(x, x)
#a = x.sum().detach() #equivalent to a = 6
a = x.sum() # here a is a function of x
g = (f-a)**2
g.backward()
print(x.grad)
```

```
tensor([-44., 132., 308., 484.])
```

De-activating the autograd engine

- If you want to avoid calculating gradients, you can use torch.no_grad() to de-activate the autograd engine.
- This will reduce memory usage and speed up computations but you won't be able to backprop (which you don't want in an eval script).

In [6]:
```
x = torch.arange(4.0)
x.requires_grad_(True)
with torch.no_grad():
    f = 2*torch.dot(x, x)
print(f) # the forward pass i.e. the value of f is calculated as normal
f.backward() # the backward pass will throw an error
```

```
tensor(28.)

---------------------------------------------------------------------------
RuntimeError                              Traceback (most recent call last)
<ipython-input-6-dbf5ed6d017d> in <module>
      4     f = 2*torch.dot(x, x)
      5 print(f) # the forward pass i.e. the value of f is calculated as norma
l
----> 6 f.backward() # the backward pass will throw an error

~/miniconda3/lib/python3.7/site-packages/torch/tensor.py in backward(self, gra
dient, retain_graph, create_graph)
    183                 products. Defaults to ``False``.
    184         """
--> 185         torch.autograd.backward(self, gradient, retain_graph, create_g
```

Summary

- A derivative can be interpreted as the instantaneous rate of change of a function with respect to its variable.
- It is also the slope of the tangent line to the curve of the function.
- A gradient is a vector whose components are the partial derivatives of a multivariate function with respect to all its variables.
- The chain rule enables us to differentiate composite functions.
- Deep learning frameworks overcome this problem by automatically calculating derivatives, by *automatic differentiation*.
- Automatic differentiation enables the system to subsequently calculate gradients.