lecture_10_optimisation_ii

April 21, 2021

1 Lecture 10: Optimisation II

1.1 Data Science Fundamentals

1.2 ## Parameters, objective functions, classification of optimisation problems

DSF - University of Glasgow - Chris McCaig - 2020/2021

2 Summary

By the end of this unit you should know: * basic uses of optimisation and how to come up with objective functions * what linear least squares is * how iterative optimisation works * the principles of heuristic optimisation * the properties of random search, with the metaheuristics: locality, memory, temperature and population* what first-order optimisation is * how gradient descent works * what automatic differentiation is, and why it is important for optimisation * what the Jacobian (matrix), gradient (vector) and Hessian (matrix) are, and how they characterise the local behaviour of the objective function * what continuity is, and how Lipschitz continuity relates to gradient descent * how stochastic relaxation can be used to create smooth continuous objective functions from discontinuous ones * what stochastic gradient descent is and why it is useful * what momentum is, and how it can improve gradient descent * what second-order methods are and their limitations

[1]:
```
import IPython.display
IPython.display.HTML("""
<script>
  function code_toggle() {
    if (code_shown){
      $('div.input').hide('500');
      $('#toggleButton').val('Show Code')
    } else {
      $('div.input').show('500');
      $('#toggleButton').val('Hide Code')
    }
    code_shown = !code_shown
  }

  $( document ).ready(function(){
    code_shown=false;
```

```
    $('div.input').hide()
  });
</script>
<form action="javascript:code_toggle()"><input type="submit" id="toggleButton"␣
 ↪value="Show Code"></form>""")
```

[1]:
```
<IPython.core.display.HTML object>
```

[13]:
```
from __future__ import print_function, division
import numpy as np
import matplotlib as mpl

import scipy.optimize    # scipy's optimisation routines
%matplotlib inline
import matplotlib.pyplot as plt
plt.rc('figure', figsize=(8.0, 4.0), dpi=140)
from utils.history import History, linear_regression_plot

# loss function
def loss(theta):
    # sum of squares of differences with estimated parameters
    e = np.sum(((line_x * theta[0] + theta[1]) - line_y) ** 2)
    return e
```

3 Metaheuristics

There are a number of standard **meta-heuristics** than can be used to improve random search.

These are: * **Locality** which takes advantage of the fact the objective function is likely to have similar values for similar parameter configurations. This assumes *continuity* of the objective function. * **Temperature** which can change the rate of movement in the parameter space over the course of an optimisation. This assumes the existence of local optima. * **Population** which can track multiple simultaneous parameter configurations and select/mix among them. * **Memory** which can record good or bad steps in the past and avoid/revisit them.

3.1 Locality

Local search refers to the class of algorithms that make *incremental* changes to a solution. These can be much more efficient than random search or grid search when there is some continuity to the objective function. However, they are subject to becoming trapped in **local minima**, and not reaching the **global minimum**. Since they are usually exclusively used for nonconvex problems, this can be a problem.

This implies that the output of the optimisation depends on the **initial conditions**. The result might find one local minimum starting from one location, and a different local minimum from another starting parameter set.

Local search can be thought of forming **trajectory** (a path) through the parameter space, which should hopefully move from high loss towards lower loss.

3.1.1 Hill climbing: local search

Hill climbing is a modification of random search which assumes some topology of the parameter space, so that there is a meaningful concept of a **neighbourhood** of a parameter vector; that we can make incremental changes to it. Hill climbing is a form of **local search**, and instead of drawing samples randomly from the parameter space, randomly samples configurations *near* the current best parameter vector. It makes incremental adjustments, keeping transitions to neighbouring states only if they improve the loss.

Simple hill climbing adjusts just one of the parameter vector elements at a time, examining each "direction" in turn, and taking a step if it improves things. **Stochastic hill climbing** makes a random adjustment to the parameter vector, then either accepts or rejects the step depending on whether the result is an improvement.

The name *hill climbing* comes from the fact that the algorithm randomly wanders around, only ever taking uphill (or downhill, for minimisation) steps. Because hill climbing is a **local search** algorithm, it is vulnerable to getting stuck in local minima. Basic hill climbing has no defence against minima and will easily get trapped in poor solutions if they exist. Simple hill climbing can also get stuck behind **ridges** and all forms of hill climbing struggle with **plateaus** where the loss function changes slowly.

Pros

- Not much more complicated than random search
- Can be *much* faster than random search

Cons

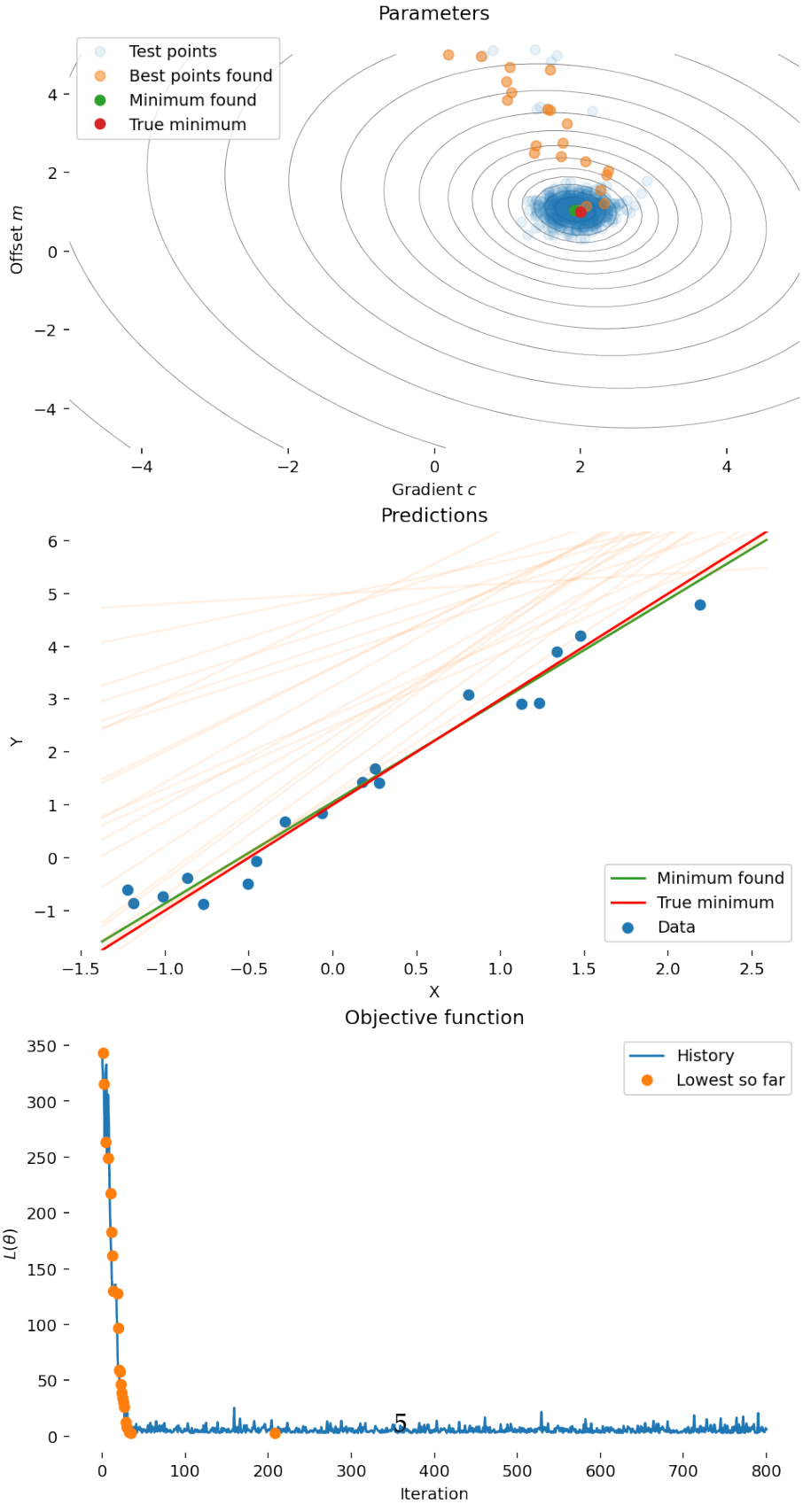
- Hard to choose how much of an adjustment to make
- Can get stuck in minima
- Struggles with objective function regions that are relatively flat
- Requires that the objective function be (approximately) continuous

[2]:
```
def stochastic_hill_climbing(L, guess_fn, neighbour_fn, iters):
    """
    L: loss function
    theta_0: initial guess
    neighbour_fn(theta): given a parameter vector, returns a random vector nearby
    iters: number of iterations to run the optimisation for
    """
    o = History()
    theta_0 = guess_fn()
    o.track(theta_0, L(theta_0))
    for i in range(iters):
        proposal = neighbour_fn(o.best_theta)
        o.track(proposal, L(proposal))
    return o.finalise()
```

[3]:
```
line_x = np.sort(np.random.normal(0, 1, (20,)))
gradient, offset = 2, 1  # these are the "true" parameters that generated this␣
 ↪data
# 2x + 1 and a bit of noise
line_y = (
    gradient * line_x + offset + np.random.normal(0, 0.5 * np.abs(line_x),␣
 ↪line_x.shape)
)

def sample():
    # guess
    return np.random.normal(0,5,size=(2,))

def neighbour(x):
    # adjust the guess a bit
    return np.random.normal(0,0.25,x.shape) + x


hill_results = stochastic_hill_climbing(loss, sample, neighbour, 800)
```

[4]:
```
linear_regression_plot(hill_results, gradient, offset, line_x,line_y, "Hill␣
 ↪climbing search")
```

Hill climbing search over possible line configurations



Again, there are many ways this basic algorithm can be tweaked: * **adaptive local search** where the size of the neighbourhood can be adapted (e.g. if no improvement in n iterations, increase size of random steps) * **multiple restarts** can be used to try and avoid getting stuck in local minima by running the process several times for random initial guesses. This is another meta-heuristic – a heuristic applied to the search algorithm itself.

3.2 Temperature

3.2.1 Simulated annealing: temperature schedules and minima escaping

Simulated annealing extends hill-climbing with the ability to sometimes randomly go uphill, instead of always going downhill. It uses a **temperature schedule** that allows more uphill steps at the start of the optimisation and fewer ones later in the process. This is used to overcome ridges and avoid getting stuck in local minima.

The idea is that allowing random "bad jumps" early in a process can help find a better overall configuration.

Image: hill climbing would get stuck in the local minimum at the left. Simulated annealing would sometimes accept "bad" local changes to ride over hills and get to a better minimum.

The "temperature schedule" comes from the idea of **annealing** metals. Molten metals have molecules bouncing around all over the place. As they cool, the random bouncing gets smaller and smaller as the molecules lock together into a tight lattice. Fast cooling results in less well structured metals than slow cooling.

3.2.2 Accepting you have to go uphill sometimes

Simulated annealing uses the idea of **acceptance probability**. Instead of just accepting any random change that decreases the loss, we randomly accept some proportion of jumps that might temporarily increase the loss, and slowly decrease the proportion of these over time.

Given the current loss $l = L(\theta)$ and a proposed new loss $l' = L(\theta + \Delta\theta)$, where $\Delta\theta$ represents a random perturbation of θ, we can define a probability $P(l, l', T(i))$ which is the probability of jumping from θ to $\Delta\theta$ at iteration i.

A common rule is: * $P(l, l', T(i)) = 1$ if $l' < l$, i.e. always go downhill. * $P(l, l', T(i)) = e^{-(l-l')}T(i)$ i.e. take uphill jumps if the relative decrease is small.

$T(i)$ is typically an exponentially decaying function of the iteration number, so that large jumps are accepted at the start, even if they go *way* uphill, but there is a decreasing tendency to make uphill jumps as time goes on.

For example,

$$T(i) = e^{\frac{-i}{r}},$$

where i is the iteration number, r is the cooling rate and T is the temperature.

[Image: By Kingpin13 - Own work, CC0, [from Wikipedia(https://commons.wikimedia.org/w/index.php?curid=25010763)]

It was originally invented to help design VLSI chip layouts and routing at IBM. IBM engineers had a few "gurus" who knew how to map out "good paths" on the silicon, and they couldn't keep up with the layout demand. The annealing procedure was introduced to find good routings automatically. It was better than the gurus were. And cheaper too.

Pros

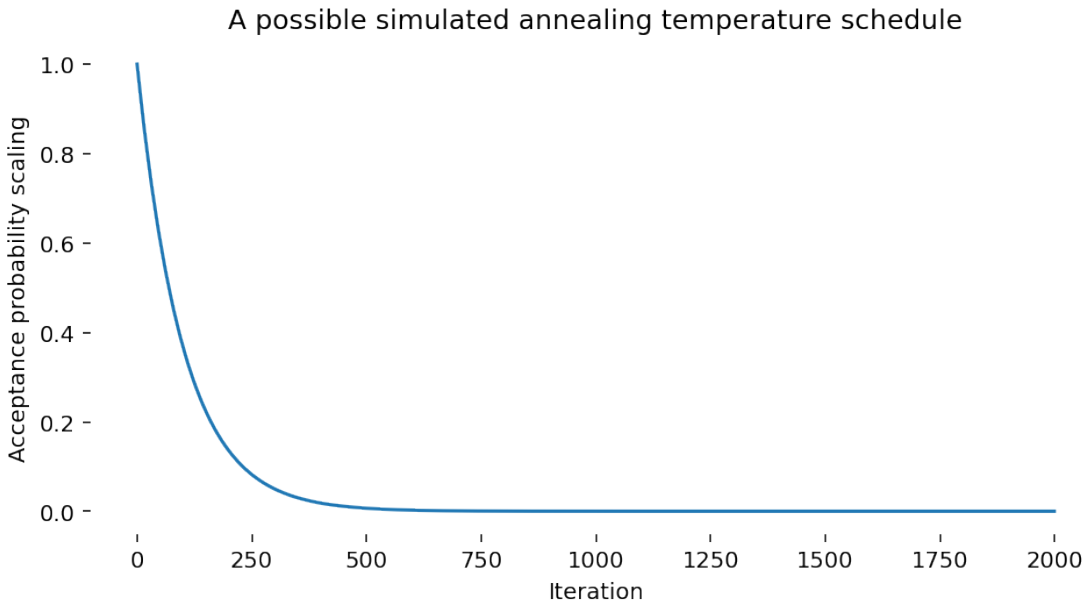
- Much less sensitive to getting trapped in minima than hill climbing
- Easy to implement
- Empirically very effective
- Fairly effective even in mixed continuous/discrete settings.

Cons

- Depends on good choice for the temperature schedule and neighbourhood function, which are extra free parameters to worry about.
- No guarantees of convergence
- Slow if the uphill steps are not actually needed

[5]:
```
import numpy as np
def temperature(iteration):
    return np.exp(-iteration/100.0)

iterations = np.arange(2000)
fig = plt.figure()
ax = fig.add_subplot(1,1,1)
ax.plot(iterations, temperature(iterations))
ax.set_xlabel("Iteration")
ax.set_ylabel("Acceptance probability scaling")
ax.set_frame_on(False)
ax.set_title("A possible simulated annealing temperature schedule")
```

[5]:
```
Text(0.5, 1.0, 'A possible simulated annealing temperature schedule')
```

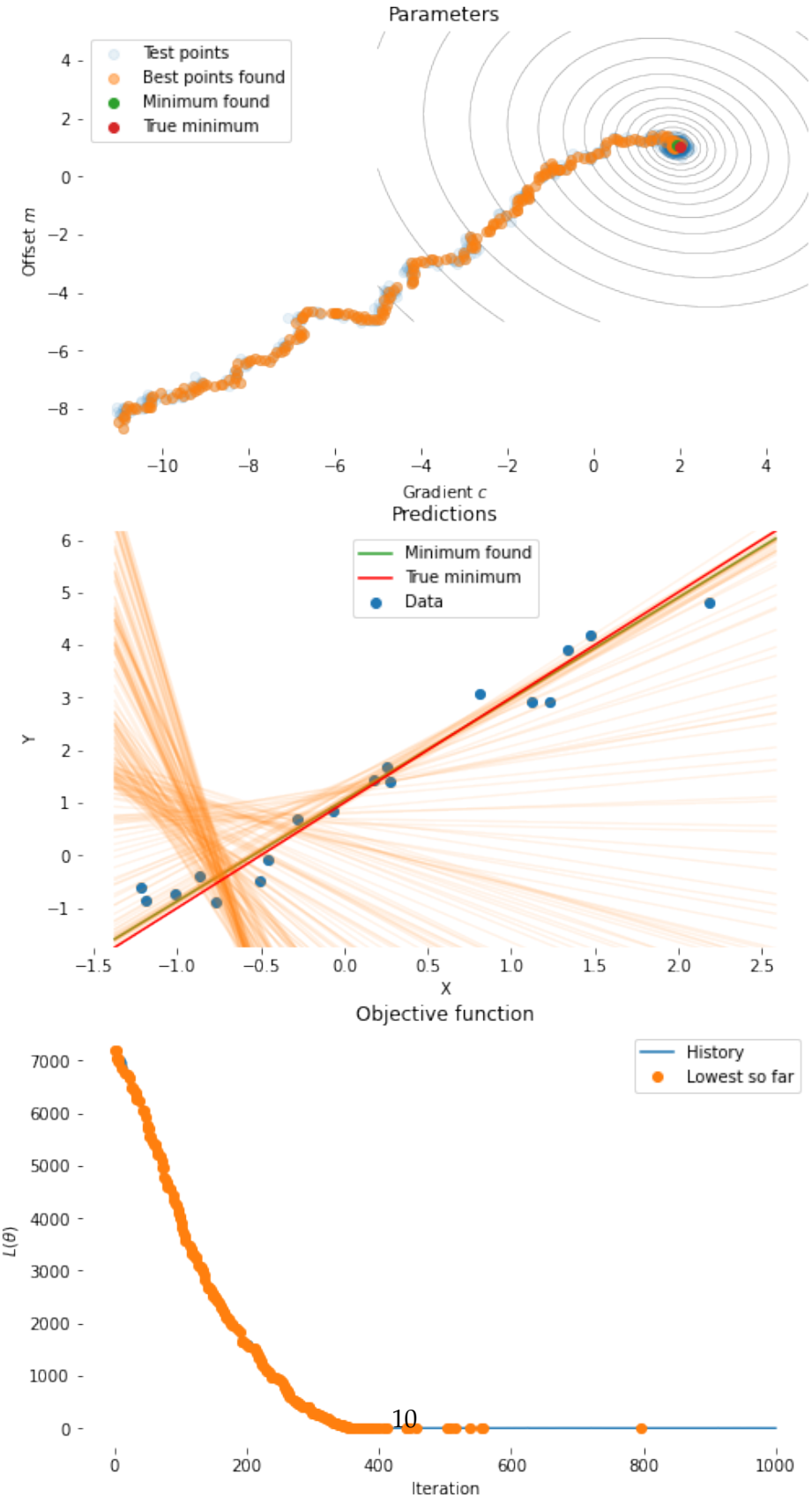


[6]:
```
def simulated_anneal(L, guess_fn, neighbour_fn,
                     temperature_fn, iters):
    """
    L: loss function
    guess_fn: function that should return an initial guess
    neighbour_fn(theta): given a parameter vector,
                         returns a random vector nearby
    temperature_fn(iter): given an iteration,
                          return the temperature schedule
    iters: number of iterations to run the optimisation for
    """
    o = History()
    theta_0 = guess_fn()
    o.track(theta_0, L(theta_0))
    state = theta_0.copy()
    loss = L(theta_0)
    for i in range(iters):
        proposal = neighbour_fn(state)
        proposal_loss = L(proposal)
        # climb if we can
        if proposal_loss<loss:
            o.track(proposal, proposal_loss, force=True)
            loss, state = proposal_loss, proposal

        else:
            # check how bad this jump might be
```

```
            p = np.exp(-(proposal_loss-loss)) * temperature_fn(i)
            # randomly accept the jump with the given probability
            if np.random.uniform(0,1)<p:
                o.track(proposal, proposal_loss, force=True)
                loss, state = proposal_loss, proposal
            else:
                o.track(proposal, proposal_loss)
    return o.finalise()
```

[7]:
```
%matplotlib inline

def sample():
    # guess
    return np.random.normal(0,5,size=(2,))

def neighbour(x):
    # adjust the guess a bit
    return np.random.normal(0,0.1,x.shape) + x

def temperature(iteration):
    return np.exp(-iteration/100.0)

anneal_results = simulated_anneal(loss, sample, neighbour, temperature, 1000)
linear_regression_plot(anneal_results, gradient, offset, line_x, line_y,␣
 ↪"Simulated annealing search")
```

Simulated annealing search over possible line configurations



[ ]:

3.2.3 More complicated example: finding evenly spaced points

This isn't very impressive for the line fitting, which is a very simple convex function; there are no local minima to get trapped in. We can look at the problem of finding a collection of points that are evenly spaced. This is non-convex (and has an infinite number of equal minima), and much harder to solve than fitting a line to some points.

This is a task particularly suited to simulated annealing-style approaches.

[8]:
```
from evenspace import pt_fit_loss, pt_fit_plot

def pt_neighbour(x):
    return x + np.random.normal(0, 0.005, x.shape)

def pt_guess():
    return np.random.uniform(0,1, (64,2)).ravel()

def pt_temperature(iteration):
    return np.exp(-iteration/1000.0)

res = simulated_anneal(lambda x:pt_fit_loss(x, shape=(64,2)), pt_guess,␣
 ↪pt_neighbour, pt_temperature, 10000)
```

[10]:
```
# # animate the result
# %matplotlib notebook
# %matplotlib notebook
# import matplotlib.pyplot as plt

# plt.figure(figsize=(8,8))
# pt_fit_plot(res, (64,2), temperature_fn=pt_temperature, title="Simulated␣
 ↪Annealing")
```

[11]:
```
# # restore normal plotting
# %matplotlib inline
# import matplotlib.pyplot as plt
# plt.rc('figure', figsize=(8.0, 4.0), dpi=140)
```

3.3 Population

Another nature-inspired variant of random search is to use a **population** of multiple competing potential solutions, and to apply some analogue of **evolution** to solving optimisation. This involves some of:

- **mutation** (introducing random variation)

- **natural selection** (solution selection)
- **breeding** (interchange between solutions)

This class of algorithms are often called **genetic algorithms** for obvious reasons. All genetic algorithms maintain some population of potential solutions (a set of vectors $\vec{\theta_1}, \vec{\theta_2}, \vec{\theta_3}, \ldots$), and some rule which is used to preserve some members of the population and cull others. The parameter set is referred to as the **genotype** of a solution.

Simple population approaches simply use small random perturbations and a simple selection rule like "keep the top 25% of solutions, ordered by loss". Each iteration will perturb the solutions slightly by random mutation, cull the weakest solutions, then copy the remaining "fittest" solutions a number of times to produce the offspring for the next step. The population size is held constant from iteration to iteration. This is just random local search with population. The idea is that this can explore a larger area of the space than simple local search and maintain multiple possible hypotheses about what might be good during that time.

Crossover rules More advanced algorithms introduce some form of **breeding** or **crossover**. David Mackay's chapter "Why have Sex? Information Acquisition and Evolution" explains some of the motivation for introducing sexual reproduction. Crossover introduces some combination of the fittest solutions as the next iteration (sexual reproduction), instead of simply copying the "parents" (asexual reproduction).

In other words, crossover "merges" two possible parameter vectors θ_{mum} and θ_{dad} to form a new child parameter θ_{baby} (although of course we are not limited to just two sexes). Crossover works well when the parameter vector can be partitioned into distinct components, where offspring can plausibly inherit good qualities from both parents. It works less well when the crossover simply becomes a mishmash of parent qualities which average out.

Genetic algorithms have been used for many practical problems which are hard to solve with existing techinques, like antenna design for spacecraft.

Image: The 2006 NASA ST5 spacecraft antenna. This complicated shape was found by an evolutionary computer design program to create the best radiation pattern. Source: Wikipedia, public domain

There is a very interesting article on Damn Interesting about a genetic algorithm which "learned" to use a subtle hardware feature the designers didn't even know about to optimise a circuit; an example of how the general approach of optimisation can help solve problems without expert insight.

Animation from Flexible Muscle-Based Locomotion for Bipedal Creatures Geijtenbeek, T., van de Panne, M. & Stappen, A.F. van der (2013)

There are *many, many* variations of genetic algorithms, including isolating populations to get "island-like" specialised selection, variable mutation rates, hybrid simulated annealing approaches, and so on.

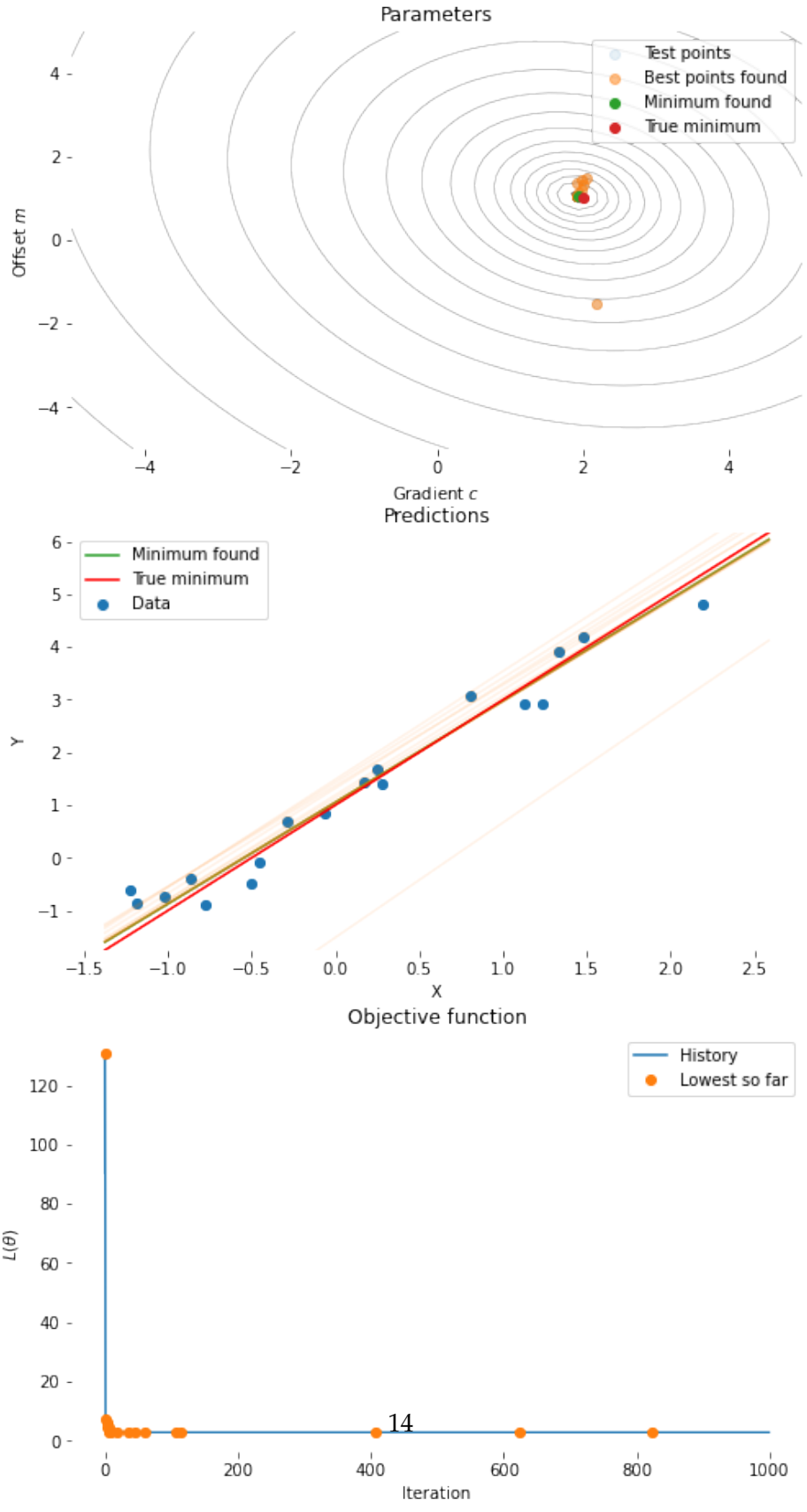
[9]:
```
def genetic_search(L, pop, guess_fn, mutation_fn, iters, keep=0.25):
    o = History()
    # create the initial population randomly
    population = np.array([guess_fn() for i in range(pop)])
    d = len(guess_fn()) # store dimensionality of problem
```

```
    loss = np.zeros(pop)

    for i in range(iters):
        for j in range(pop):
            # could also mutate *everyone* here
            # this works better in asexual reproduction
            loss[j] = L(population[j])

        # order by loss
        order = np.argsort(loss)
        loss = loss[order]
        population = population[order]

        # replicate top "keep" fraction of individuals
        top = int(pop * keep)
        for j in range(top, pop):
            # sexual reproduction
            mum = np.random.randint(0, top)
            dad = np.random.randint(0, top)
            chromosones = np.random.randint(0,2,d)

            # select elements from each dimension randomly from mum and dad
            population[j]  = mutation_fn(np.where(chromosones==0,␣
↪population[mum], population[dad]))

        # track the best individual so far
        o.track(population[0], loss[0])
    return o.finalise()
```

[10]:
```
%matplotlib inline
ga_results = genetic_search(loss, 20, sample, neighbour, 1000)
print(ga_results)
linear_regression_plot(ga_results, gradient, offset, line_x, line_y, "GA search")
```

```
<utils.history.History object at 0x00000243DBE27160>
```

GA search over possible line configurations



[11]:
```
# animate the result
%matplotlib notebook
%matplotlib notebook
import matplotlib.pyplot as plt

# do GA search this time
res = genetic_search(lambda x:pt_fit_loss(x, (64,2)), 50, pt_guess,␣
 ↪pt_neighbour, 500)

# plot the results
#pt_fit_plot(res, (64,2),  title="Genetic Algorithm")
```

3.3.1 Genetic algorithms: population search

Pros

- Easy to understand and applicable to many problems.
- Requires only weak knowledge of the objective function
- Can be applied to problems with both discrete and continuous components.
- Some robustness against local minima, although hard to control.
- Great flexibility in parameterisation: mutation schemes, crossover schemes, fitness functions, selection functions, etc.

Cons

- Many, many "hyperparameters" to tune which radically affect the performance of the optimisation. How should you choose them?
- No guarantee of convergence; *ad hoc*.
- (Very) slow compared to using stronger knowledge of the objective function.
- Many evaluations of objective function are required: one per population member per iteration.

3.4 Memory

The optimisation algorithms we have seen so far are **memoryless**. They investigate some part of the solution space, check the loss, then move on. They may end up checking the same, or very similar, solutions over and over again. This inefficiency can be mitigated using some form of **memory**, where the optimiser remembers where "good" and "bad" bits of the parameters space are, and makes decisions using this memory. In particular, we want to remember good **paths in solution space**.

3.5 Memory + population

3.5.1 Ant colony optimisation

.Original Image (without the meme text!) by Sam Droege shared public domain

Ants are really good at finding food (exploration), and then leading the whole colony to the food source to explore and extract all of the food (exploitation). They do this, without requiring any complex coordination. Instead, ants wander about until they find something to eat. Then, they leave a trail of *pheromones* (smells) behind them and wander back to the anthill. Other ants can follow this trail to find the food and check the whole area for any really tasty bits.

Ant colony optimisation combines memory and population heuristics. It uses the idea of **stigmergy** to optimise problems:

> **stigmergy**: A mechanism of spontaneous, indirect coordination between agents or actions, where the trace left in the environment by an action stimulates the performance of a subsequent action. [wiktionary.org]

.***Stigmergy*** *explains how termites are able to construct vast, sophisticated "buildings" to live in despite their tiny brains. Image by david55king shared CC BY*

In terms of optimisation this means: * having a population of parameter sets ("ants") * having a memory of good paths through the space ("pheromones")

Ants who find good parts of the space (i.e. low objective function) leave a trail of positive "pheromones", by storing marker vectors. Other ants will move towards those pheromones, and eventually follow paths that lead to good solutions. Over time (i.e. as iterations increase), the pheromones evaporate so that the ants don't get constrained into one tiny part of the space. Instead of using the physical environment, we use auxiliary data structures to memorise good paths through the parameter space, to avoid repetitious searching.

ACO is particularly well suited to path-finding and route-finding algorithms, where the memory structure of the pheromone trail corresponds to the solution structure.

Pros

- Can be very effective in spaces where good solutions are separated by large, narrow valleys.
- Can use fewer evaluations of the objective function than genetic algorithm if pheromones are effective.
- When it works, it really works.

Cons

- Moderately complex algorithm to implement.
- No guarantee of convergence; *ad hoc*.
- Even *more* hyperparameters than genetic algorithms.
- People think you work with ants.

---

4 Quality of optimisation

4.1 Convergence

An optimisation algorithm is said to **converge** to a **solution**. In convex optimisation, this means that the **global minimum** has been found and the problem is solved. In non-convex optimisation, this means a **local minimum** has been found from which the algorithm cannot escape.

A good optimisation algorithm converges quickly. This means that the drop in the objective function should be steep, so that each iteration is making a big difference. A bad optimisation algorithm does not converge at all (it may wander forever, or diverge to infinity). Many optimisation algorithms only converge under certain conditions; the convergence depends on the initial conditions of the optimisation.

4.1.1 Guarantees of convergence

Some optimisation algorithms are guaranteed to converge if a solution exists; while others (like most heuristic optimisation algorithms) are not guaranteed to converge even if the problem has a solution. For example, a random search might wander the space of possibilities forever, never finding the specific configuration that minimises (or even reduces) the loss.

For iterative solutions, a plot of the objective function value against iteration is a helpful tool in diagnosing convergence problems. Ideally, the loss should drop as fast as possible.

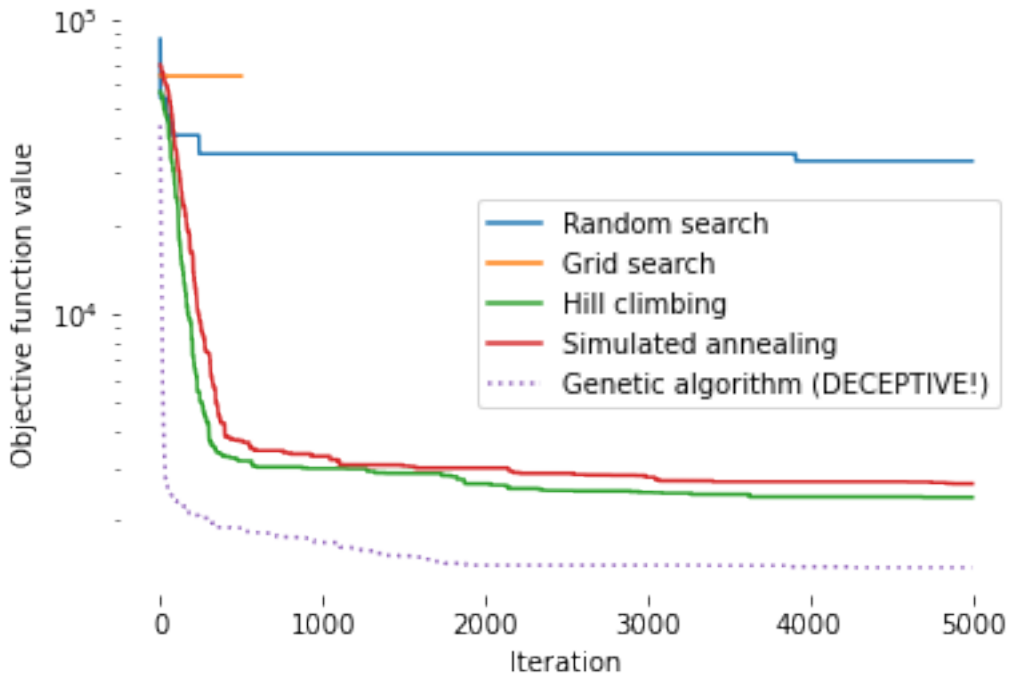
4.2 Example

This example shows the linear regression problem with the heuristic methods and gradient descent (which is *much* faster). This problem is convex and has no local minima, so hill climbing and simulated annealing have similar performance.

[12]:
```
#from autograd import grad
from utils.optimisers import random_search, grid_search, hill_climbing,␣
 ↪simulated_anneal, gradient_descent, genetic_search


# the linear regression problem; find m and c in the equation y=mx+c
dim = 30
x = np.sort(np.random.normal(0,1,(20,dim)))
A = np.random.normal(0,1,(dim,dim))
b = np.random.normal(0,10,(dim,))

y = (x@A) + b + np.random.normal(0, 0.5*np.abs(x), x.shape)
l = len(A.ravel())
params = l + len(b)
%matplotlib inline
%matplotlib inline

import matplotlib.pyplot as plt

def loss(theta):
    # sum of squares
    Ap = theta[:l].reshape(A.shape)
    bp = theta[l:]
    e = np.sum(((x @ Ap + bp) - y)**2)
    return e
```

```
# compute derivative (in one step!)
#dloss = grad(loss)

guess = lambda: np.random.normal(0,1, params)
neighbour = lambda x: x+np.random.normal(0,0.1, params)

random_res = random_search(loss, guess, 5000)
grid_res = grid_search(loss, [[-1,-1.5] for i in range( params)],
                       10, maxiter=500)
hill_res = hill_climbing(loss, guess, neighbour, 5000)

ga_res = genetic_search(loss, 50, guess, neighbour, 5000)

def temperature(iteration):
    return np.exp(-iteration/100.0)

anneal_res = simulated_anneal(loss, guess, neighbour, temperature, 5000)
#gd_res = gradient_descent(loss, dloss, guess(), 1e-3, maxiter=5000)

fig = plt.figure()
ax = fig.add_subplot(1,1,1)
ax.plot(random_res.loss_trace, label="Random search")
ax.plot(grid_res.loss_trace, label="Grid search")
ax.plot(hill_res.loss_trace, label="Hill climbing")
ax.plot(anneal_res.loss_trace, label="Simulated annealing")
#ax.plot(gd_res.loss_trace, label="Gradient descent")
ax.plot(ga_res.loss_trace, label="Genetic algorithm (DECEPTIVE!)", ls=':')
ax.set_frame_on(False)
ax.set_yscale("log")
ax.legend()
ax.set_xlabel("Iteration")
ax.set_ylabel("Objective function value")
```

[12]: `Text(0, 0.5, 'Objective function value')`



4.3 Tuning optimisation

Optimisation turns specific problems into ones that can be solved with a general algorithm, as long as we can write down an objective function. However, optimisation algorithms have **hyperparameters**, which affect the way in which the search for the optimum value is carried out. Using optimisers effectively requires adjusting these hyperparameters.

4.3.1 Use the right algorithm

- If you know the problem is **least-squares** use a specialised least-squares solver. You might be able to solve directly, for example with the pseudo-inverse.
- If you know the problem is **convex**, use a convex solver. This is radically more efficient than any other choice if its applicable.
- If you know the derivatives of the objective function, or can compute them using automatic differentiation, use a **first-order** method (or second order, if you can)
- If you don't know any of these things, use a general purpose **zeroth-order** solver like **simulated annealing** or a **genetic algorithm**.

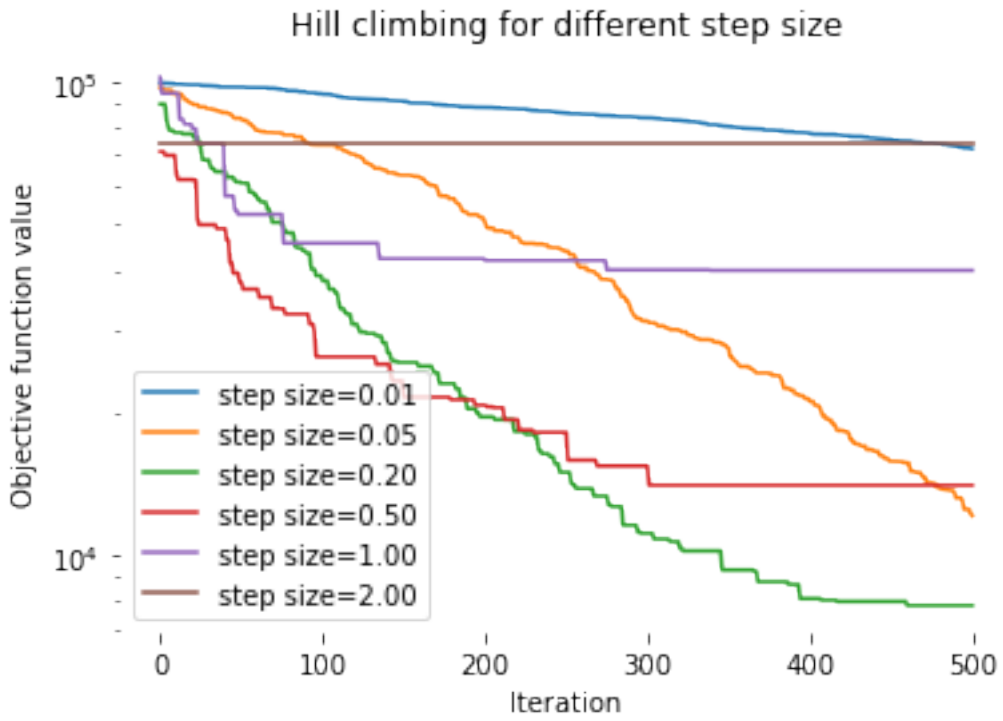
4.3.2 What can go wrong?

Slow progress Slow progress typically occurs in local search where the steps made are too small. For example, gradient descent with a very small δ or hill climbing with a tiny neighbourhood function will only be able to search a very small portion of the space. This will correspond to a very slowly decreasing loss plot.

Noisy and diverging performance Local search can also become unstable, particularly if jumps or steps are too large an the optimiser bounces around hopelessly. The optimisation can diverge if the objective function has infinitely decreasing values in some direction ("the abyss"), and this typically requires constraints to limit the **feasible set**.

[16]:
```
fig = plt.figure()
ax = fig.add_subplot(1,1,1)

for step in [0.01, 0.05, 0.2, 0.5, 1.0, 2.0]:
    hill_res = hill_climbing(loss, lambda: np.random.normal(0,1, params),
                             lambda x: x+np.random.normal(0,step, params), 500)

    ax.plot(hill_res.loss_trace, label="step size=%.2f" % step)
ax.set_yscale("log")
ax.legend()
ax.set_xlabel("Iteration")
ax.set_frame_on(False)
ax.set_ylabel("Objective function value")
ax.set_title("Hill climbing for different step size")
```

[16]:
```
Text(0.5, 1.0, 'Hill climbing for different step size')
```



4.3.3 Getting stuck

Some optimisers can get stuck, usually at critical points of the objective function. * **Plateaus** can cause memoryless algorithms to wander, and derivative-based algorithms to cease moving entirely. Techniques like **momentum** and other forms of **memory** can limit this effect. * **Local minima** can completely trap pure local search methods and halt progress. Some metaheuristics, like random restart can mitigate this. * **Saddle points** can trap or slow gradient descent methods, which have trouble finding the *best* direction to go in when the function is increasing in some directions and decreasing in others. * **Very steep or discontinuous** objective functions can produce insurmountable barriers for gradient descent. Stochastic methods, like stochastic gradient descent, can "blur out" these boundaries and still make progress.

4.4 Dreaming of unseen images

Image: ***synthetic*** *celebrity faces, dreamed up in the imagination of a deep neural network. From: Progressive Growing of GANs for Improved Quality, Stability, and Variation Tero Karras, Timo Aila, Samuli Laine, Jaakko Lehtinen Submitted to ICLR 2018*

Cool video

5 Example: deep neural networks

Deep learning or **deep neural networks** have become a major part of modern machine learning research. They have had astonishing success in fields like speech recognition, machine translation, image classification and image synthesis. The basic problem of deep learning is one of finding an approximating function. In a simple model, this might work as follows: Given some observations $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$ and some corresponding outputs $y_1, y_2, \ldots, y_n$, find a function $y' = f(\vec{x}; \theta)$ with parameters θ, such that we have

$$\theta^* = \texttt{argmin}_\theta \sum_i ||f(\vec{x}_i; \theta) - y_i||$$

where distance is some measure of how close the output of f and the expected output y_i are (the specific distance used varies with the problem). The idea is that we can learn f such that we can generalise the transform to $\vec{x}$ we haven't seen yet. This is obviously an optimisation problem. But deep neural networks can have *tens of millions* of parameters - a very long θ vector. How is it possible to do optimisation in reasonable time in such a large parameter space? *The example above has tens of millions of parameters that need to be adjusted.*

5.0.1 Backpropagation

Origami Hummingbird by Brett Jordan is licensed under CC BY 2.0 Rotating, translating and a simple, fixed fold can form space into arbitrarily complex shapes.

The answer is that these networks are constructed in a very simple (but clever way). A traditional neural network consists of a series of **layers**, each of which is a **linear map** (just a matrix multiply) followed by a simple, fixed nonlinear function. Think: rotate, stretch (linear map) and fold (simple *fixed* nonlinear folding). The output of one layer is the input for the next.

Image: a 3 layer deep network. Each layer consists of a linear map W applied to the input x from the previous layer, followed by a fixed nonlinear function $G(\vec{x})$

The linear map in each layer is (of course) specified by a matrix, known as the **weight matrix**. The network is completely parameterised by the entries of the weight matrices for each layer (all of the entries of these matrices can be seen as the parameter vector θ). The nonlinear function $G(\vec{x})$ is fixed for every layer and cannot vary; it is often a simple function which "squashes" the range of the output in some way (like `tanh`, `relu` or `sigmoid` – you don't need to know these). Only the weight matrices change during optimisation.

$$\vec{y}_i = G(W_i\vec{x}_i + \vec{b}_i)$$

[2]:
```
# here is a neural network

# compute the prediction (output) of a
# deep neural network
# given a list of weight matrices

def G(x):
    return np.maximum(x, 0) # ReLU

def predict(x, weights, biases):
    for b_i, w_i in zip(biases, weights):
        x = G(w_i @ x + b_i)
    return x

# "all" we have to do is adjust "weights" and
# "biases" until we get the result we want :)
# These are our parameter vector, theta

def train(x, y, w_shapes, b_shapes):
    #???
    pass
```

And this particular construction (under certain conditions) has the massive advantage that the **derivative** of the objective function *with respect to the weights* can be computed for every weight in the network at the same time, even when multiple layers are composed together. The algorithm that does is called *backpropagation* and it is an algorithm for **automatic differentiation**. The "derivative with respect to the weights" means that we can tell how much of an effect each weight will have on the prediction, for every weight in the whole network, in one go.

If we imagine all of the elements of the weight matrices concatenated into a single vector θ, we can get the **gradient** of the objective function w.r.t θ. This makes the optimisation "easy"; we can just walk in the direction that takes us downhill fastest.

[*If you really want to understand what is going on in learning in deep networks, read colah's blog another colah article, and Nielsen's free book, or Deep learning from scratch]*

5.1 Why not use heuristic search?

Heuristic search methods like random search, simulated annealing and genetic algorithms are easy to understand, easy to implement and have few restrictions on the problems they can be applied to. So why not always use those approaches?

- They can be very slow; it may take many iterations to approach a minimum and require significant computation to compute each iteration.
- There is no guarantee of convergence, or even of progress. The search can get stuck, or drift slowly over plateaus.
- There are a huge number of **hyperparameters** that can be tweaked (temperature schedules, size of population, memory structure, etc.). How should these be chosen? Optimal choice of these parameters becomes an optimisation problem in itself.

For optimisation problems like deep neural networks, heuristic search is hopelessly inadequate. It is simply too slow to make progress in training networks with millions of parameters. Instead, **first-order** optimisation is applied. **First-order algorithms**, that we will discuss today, can be *orders of magnitude* faster than heuristic search.

Note: if an objective function is known to be convex with convex constraints, there are much better methods still for optimisation, which can often run exceptionally quickly with guaranteed convergence.

5.2 Rolling a ball: physical optimisation

An intuition for higher-order optimisation can be formed by considering a ball rolling on a (smooth) surface, which represents the value of the objective function across a 2D domain (i.e. if we had a parameter vector θ with two elements).

Gravity applies a force perpendicular to the plane of the surface. The surface applies a force to the ball along the direction of the *surface normal*, the vector that points "straight out" from the surface. This results in a force component in *the direction of the steepest slope* of the surface, accelerating the ball in that direction. This *gradient vector always points in the direction of the steepest slope*.

The ball will eventually settle in a configuration where there is a balanced set of forces applied to it. This will happen, for example, if the ball settles at a minimum where the normal of the surface is parallel with gravity.

5.2.1 Attractors: flowing towards a solution

We can see this as an **attractor** that draws our search towards a solution. The trajectory of the search is parallel to the "flow field" of the objective function. Our physical intuition is that we can find minima by rolling into "basins" by following these flow lines.

5.2.2 Jacobian: matrix of derivatives

- If $f(x)$ is a scalar function of a scalar x, $f'(x)$ is the first derivative of f w.r.t. x, i.e. $\frac{d}{dx}f(x)$. The second derivative is written $f''(x) = \frac{d^2}{dx^2}f(x)$.
- If we generalise this to a **vector** function $\vec{y} = f(\vec{x})$, then we have a rate of change (derivative) between every component of the input and every component of an output at any specific

input $\vec{x}$. We can collect this derivative information into a matrix called the **Jacobian matrix**, which characterises the slope *at a specific point* $\vec{x}$. If the input $\vec{x} \in \mathbb{R}^n$ and the output $\vec{y} \in \mathbb{R}^m$, then we have an $m \times n$ matrix:

$$f'(\vec{x}) = \vec{J} = \begin{bmatrix} \frac{\partial y_0}{\partial x_0} & \frac{\partial y_0}{\partial x_1} & \cdots & \frac{\partial y_0}{\partial x_n} \\ \frac{\partial y_1}{\partial x_0} & \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \cdots & & & \\ \frac{\partial y_m}{\partial x_0} & \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

This simply tells us how much each component of the output changes as we change any component of the input – the generalised "slope" of a vector-valued function. This is a very important way of characterising the variation of a vector function at a point $\vec{x}$, and is widely used in many contexts. In the case where f maps $\mathbb{R}^n \to \mathbb{R}^n$ (from a vector space to the same vector space), then we have a square $n \times n$ matrix $\vec{J}$ with which can we do standard things like compute the determinant, take the eigendecomposition or (in some cases invert).

In many cases, we have a very simple Jacobian: just one single row. This applies in cases where we have a scalar function $y = f(\vec{x})$, where $y \in \mathbb{R}$ (i.e. a one dimensional output from an n dimensional input). This is the situation we have with a loss function $L(\theta)$ is a scalar function of a vector input. In this case, we have a single row Jacobian: the gradient vector.

5.3 Gradient vector: one row of the Jacobian

- $\nabla f(\vec{x})$ is the *gradient vector* of a (scalar) function of a vector, the equivalent of the first derivative for vector functions. We have one (partial) derivative per component of $\vec{x}$. This tells us how much $f(\vec{x})$ would vary if we made tiny changes to each dimension *independently*. Note that in this course we only deal with function $f(x)$ with scalar outputs, but with vector inputs. We will work with scalar objective functions $L(\theta)$ of parameter vectors θ.

$$\nabla L(\vec{\theta}) = \left[\frac{\partial L(\vec{\theta})}{\partial \theta_1}, \frac{\partial L(\vec{\theta})}{\partial \theta_2}, \ldots, \frac{\partial L(\vec{\theta})}{\partial \theta_n}, \right]$$

- If $L(\theta)$ is a map $\mathbb{R}^n \to \mathbb{R}$, (i.e. a scalar function, like an ordinary objective function) then $\nabla L(\theta)$ is a vector valued map $\mathbb{R}^n \to \mathbb{R}^n$;
  - If $L(\theta)$ was a map $\mathbb{R}^n \to \mathbb{R}^m$, then $\nabla L(\theta)$ is matrix valued map $\mathbb{R}^n \to \mathbb{R}^{m \times n}$;

$\nabla L(\theta)$ is a vector *which points in the direction of the steepest change in* $L(\theta)$.

5.4 Hessian: Jacobian of the gradient vector

- $\nabla^2 f(\vec{x})$ is the *Hessian matrix* of a (scalar) function of a vector, the equivalent of the second derivative for vector functions.

Following our rule above, it's just the Jacobian of a vector valued function, so we know:

- $\nabla^2 L(\theta)$ is matrix valued map $\mathbb{R}^n \to \mathbb{R}^{n \times n}$

This is important, because we can see that the second derivative even of a scalar valued function scales quadratically with the dimension of its input!

(if the original function was a vector, we'd have a Hessian tensor instead).

$$H(L) = \nabla\nabla L(\vec{\theta}) = \nabla^2 L(\vec{\theta}) = \begin{bmatrix} \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1^2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1 \partial \theta_2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1 \partial \theta_3} & \cdots & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1 \partial \theta_n} \\ \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2^2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2 \partial \theta_3} & \cdots & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2 \partial \theta_n} \\ \cdots & & & & \\ \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n \partial \theta_1} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n \partial \theta_2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n \partial \theta_3} & \cdots & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n^2} \end{bmatrix},$$

5.4.1 Differentiable objective functions

For some objective functions, we can compute the (exact) **derivatives** of the objective function with respect to the parameters θ. For example, if the objective function has a single scalar parameter $\theta \in \mathbb{R}$ and the function is:

$$L(\theta) = \theta^2$$

then, from basic calculus, the derivative with respect to θ is just:

$$L'(\theta) = 2\theta.$$

If we know the derivative, we can use this to move in "good directions" – down the slope of the objective function towards a minimum.

This becomes slightly more involved for multidimensional objective functions (where θ has more than one component) where we have a **gradient vector** instead of a simple scalar derivative (written $\nabla L(\theta)$). However, the same principle applies.

Orders: zeroth, first, second Iterative algorithms can be classified according to the order of derivative they require: * a **zeroth order** optimisation algorithm only requires evaluation of the objective function $L(\theta)$. Examples include random search and simulated annealing.

- a **first order** optimisation algorithm requires evaluation of $L(\theta)$ and its derivative $\nabla L(\theta)$. This class includes the family of **gradient descent** methods.
- a **second order** optimisation algorithm requires evaluation $L(\theta)$, $\nabla L(\theta)$ and $\nabla\nabla L(\theta)$. These methods include **quasi-Newtonian** optimisation.

6 Optimisation with derivatives

If we know (or can compute) the **gradient** an objective function, we know the **slope** of the function at any given point. This gives us both: * the direction of fastest increase and * the steepness of that slope.

This is *the* major application of calculus.

Knowing the derivative of the objective function is sufficient to dramatically improve the efficiency of optimisation.

6.1 Conditions

6.1.1 Differentiability

A **smooth function** has continuous derivatives up to some order. Smoother functions are typically easier to do iterative optimisation on, because small changes in the current approximation are likely to lead to small changes in the objective function. We say a function is C^n **continuous** if the nth derivative is continuous.

Image: left-to-right, top-to-bottom discontinuous, C^0, C^1, C^2 continuous functions

There is a difference between *having continuous derivatives* and *knowing what those derivatives are*.

First order optimisation uses the (first) **derivatives of the objective function with respect to the parameters**. These techniques can only be applied if the objective function is: * At least C^1 **continuous** i.e. no step changes anywhere in the function or its derivative * **differentiable** i.e. gradient is defined everywhere

(though we will see that these constraints can be relaxed a bit in practice).

Many objective functions satisfy these conditions, and first-order methods can be vastly more efficient than zeroth-order methods. For particular classes of functions (e.g. convex) there are known bounds on number of steps required to converge for specific first-order optimizers.

6.1.2 Lipschitz continuity (no ankle breaking)

First-order (and higher-order) continuous optimisation algorithms put a stronger requirement on functions than just C^1 continuity and require the function to be **Lipschitz continuous**.

For functions $\mathbb{R}^n \to \mathbb{R}$ (i.e. the objective functions $L(\theta)$ we are concerned with), this is equivalent to saying that the *gradient is bounded* and the function cannot change more quickly than some constant; there is a maximum steepness. $\frac{\partial L(\theta)}{di} \leq K$ for all i and some fixed K.

Small Lipschitz constant *Video: the white cone never intersects the function, no matter where it is slid along the function. This function is Lipschitz continuous; the gradient is bounded everywhere, so that nowhere is steep enough that it intersects the cone.* #### Large Lipschitz constant

6.1.3 Lipschitz constant

We can imagine running a cone of a particular steepness across a surface. We can check if it ever touches the surface. This is a measure of how steep the function is; or equivalently the bound of the first derivative. The **Lipschitz constant** K of a function $f(x)$ is a measure of wide this cone that only touches the function once is. This is a measure of how smooth the function is, or equivalently the maximum steepness of the objective function at any point anywhere over its domain. It can be defined as:

$$K = \sup \left[\frac{|f(x) - f(y)|}{|x - y|} \right],$$

where sup is the supremum; the smallest value that is larger than every value of this function.

A smaller K means a function that is smoother. $K = 0$ is totally flat. We will assume that the functions we will deal with have some finite K, though its value may not be precisely known.

6.2 Analytical derivatives

If we have **analytical derivatives** (i.e. we know the derivative of the function in closed form; we can write down the maths directly), you will probably remember the "high school" process for mathematical optimisation: * compute the derivative $f'(x) = \frac{d}{dx}f(x)$ * solve for the derivative being zero (i.e. solve x for $f'(x) = 0$). This finds all **turning points** or **optima** of the function. * then check if any of the solutions has positive second derivative $f''(x) > 0$, which indicates the solution is a minimum. ### Example This is how we might find the minimum of

$$f(x) = x^4 - 40x^2 - 100x.$$

The derivative is:

$$f'(x) = 4x^3 - 80x - 100$$

and the second derivative is

$$f''(x) = 12x^2 - 80.$$

We can solve for:

$$f'(x) = 4x^3 - 20x - 100 = 0,$$

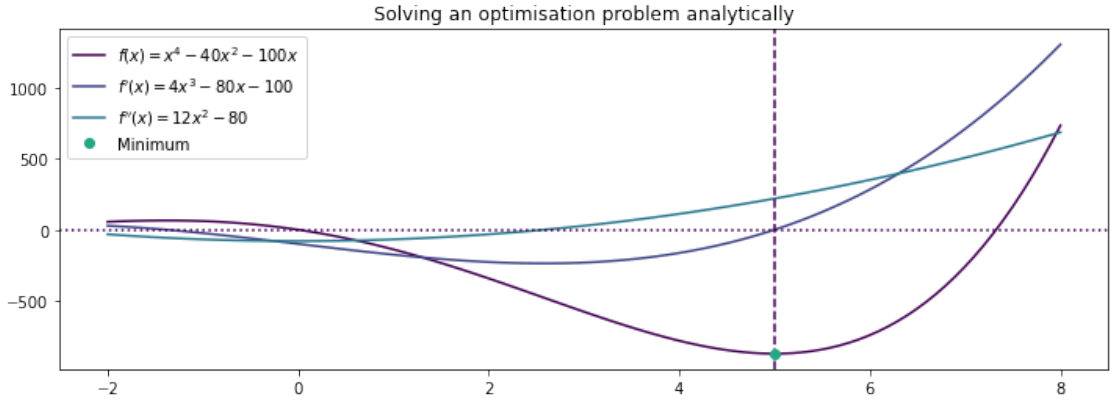
and check the sign of

$$f''(x) = 12x^2 - 20$$

to find if we have a minimum.

[359]:
```
f = lambda x:x**4 - 40*x**2 - 100*x
df = lambda x:4*x**3 - 80*x - 100
ddf = lambda x:12*x**2-80

x = np.linspace(-2,8,100)
fig = plt.figure(figsize=(12, 4))
ax = fig.add_subplot(1,1,1)
ax.plot(x, f(x), label="$f(x)=x^4 -40x^2 -100x$")
ax.plot(x, df(x), label="$f^\prime(x)=4x^3 - 80x - 100$")
ax.plot(x, ddf(x), label="$f^{\prime\prime}(x)= 12x^2 - 80$")

# solution is 5.0 by inspection
ax.axhline(0, ls=':')
ax.axvline(5.0, ls='--')
ax.plot(5.0, f(5.0), 'o', label='Minimum')
ax.legend()
ax.set_title("Solving an optimisation problem analytically")
print(df(5.0), ddf(5.0))
```

```
0.0 220.0
```



6.3 Computable exact derivatives

The analytical derivative approach doesn't require any iteration at all. We get the solution immediately on solving for the derivative. But usually we don't have a simple solution for the derivative, but we can evaluate the derivative *at a specific point*; we have **exact pointwise derivatives**. We can evaluate the function $f'(x)$ for any x but not write it down in closed form. In this case, we can still dramatically accelerate optimisation by taking steps such that we "run downhill" as fast as possible. This requires that we can compute the gradient at any point on the objective function.

6.4 Gradient: A derivative vector

We will work with objective functions that take in a vector and output a scalar:

```
# vector -> scalar
def objective(theta):
    ...
    return score
```

We want to be able to *generate* functions:

```
# vector -> vector
def grad_objective(theta):
    ...
return score_gradient
```

Mathematically, we can write the vector of derivatives as:

$$\nabla L(\vec{\theta}) = \left[\frac{\partial L(\vec{\theta})}{\partial \theta_1}, \frac{\partial L(\vec{\theta})}{\partial \theta_2}, \ldots, \frac{\partial L(\vec{\theta})}{\partial \theta_n}, \right]$$

Note: $\frac{\partial L(\vec{\theta})}{\partial \theta_1}$ just means the change in L in the direction θ_1 at the point $\vec{\theta}$.

This vector $\nabla L(\vec{\theta})$ is called the **gradient** or **gradient vector**. At any given point, the gradient of a function points in the direction where the function *increases fastest*. The magnitude of this vector is the rate at which the function is changing ("the steepness").

6.5 Gradient descent

The basic first-order algorithm is called **gradient descent** and it is very simple, starting from some initial guess $\theta^{(0)}$:

$$\theta^{(\vec{i+1})} = \theta^{(\vec{i})} - \delta \nabla L(\theta^{(\vec{i})})$$

where δ is a scaling hyperparameter – the **step size**. The **step size** might be fixed, or might be chosen adaptively according to an algorithm like *line search*.

This means is that the optimiser will make moves where the objective function drops most quickly.

In simpler terms:

- starting somewhere $\theta^{(0)}$
- repeat:
  - check how steep the ground is in each direction $v = \nabla L(\theta^{(\vec{i})})$
  - move a little step δ in the steepest direction v to find $\theta^{(\vec{i+1})}$.

Notation note: $\theta^{(\vec{i})}$ does not mean the ith power of θ but just the ith $\vec{\theta}$ in a sequence of iterations: $\vec{\theta}^{(0)}, \vec{\theta}^{(1)}, \vec{\theta}^{(2)}, \ldots$

6.5.1 Downhill is not always the shortest route

While gradient descent *can* be very fast, following the gradient is not necessarily the fastest route to a minimum. In the example below, the route from the red point to the minimum is very short. Following the gradient, however, takes a very circuitous path to the minimum.

Image: gradient descent means following the steepest slope – not always the shortest route

It is generally much faster than blindly bouncing around hoping to get to the bottom, though!

6.6 Implementing gradient descent

The implementation follows directly from the equations:

[4]:
```
import utils.history
import imp; imp.reload(utils.history)
from utils.history import History

#
# note: fixed step size isn't a good idea!

def gradient_descent(L, dL,
                     theta_0,
                     delta, tol=1e-4):
```

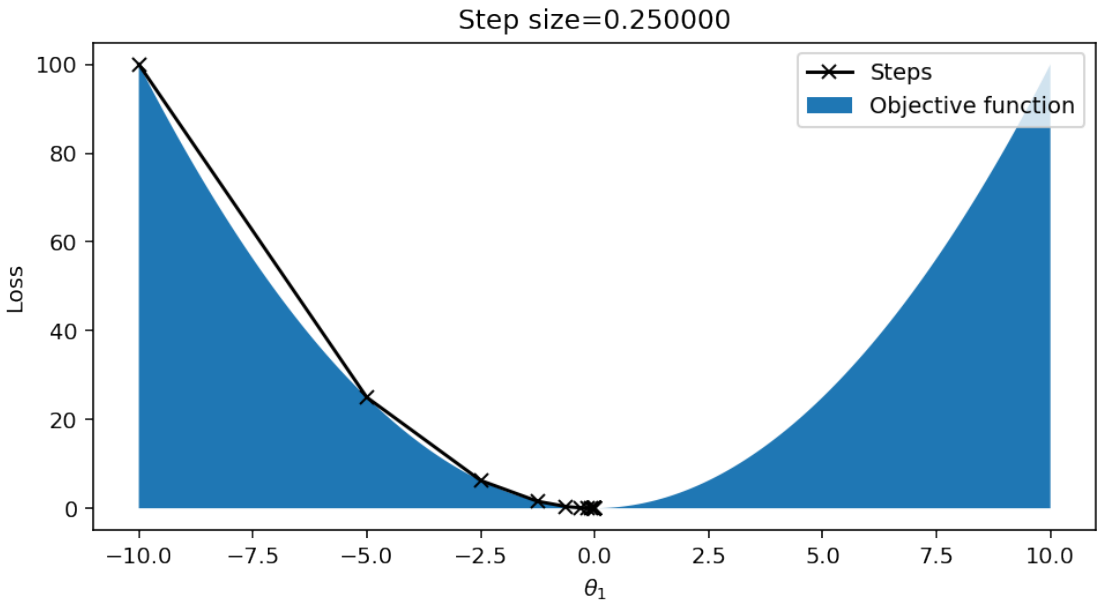
```
    """
     L: scalar loss function
     dL: gradient of loss function w.r.t parameters
     theta_0: starting point
     delta: step size
     tol: termination condition;
         when change in loss is less than tol, stop iterating
     """
    theta = np.array(theta_0) # copy theta_0
    o = History()
    o.track(np.array(theta), L(theta))

    # while the loss changes
    while np.sum(np.abs(dL(theta)))>tol:
        # step along the derivative
        theta += -delta * dL(theta)
        o.track(np.array(theta), L(theta))

    return o.finalise()
```

[24]:
```
def L(theta):
    return theta**2

def dL(theta):
    # we can differentiate L(theta) in our heads :)
    return 2*theta
```

[25]:
```
def plot_gradient_descent(xs, L, dL, x_0, step):
    # do descent
    res = gradient_descent(L, dL, x_0, step)

    # plot
    fig = plt.figure()
    ax = fig.add_subplot(1,1,1)
    ax.fill_between(xs, L(xs), label="Objective function")
    ax.set_title("Step size=%f" % step)
    ax.set_xlabel("$\\theta_1$")
    ax.set_ylabel("Loss")
    ax.plot(res.best_thetas, res.best_losses, 'k-x', label='Steps')
    ax.legend()
    print("Converged in {0} steps".format(res.iters))

xs = np.linspace(-10,10,200)
```

[26]:
```
plot_gradient_descent(xs, L, dL, [-10.], 0.25)
```

```
Converged in 19 steps
```

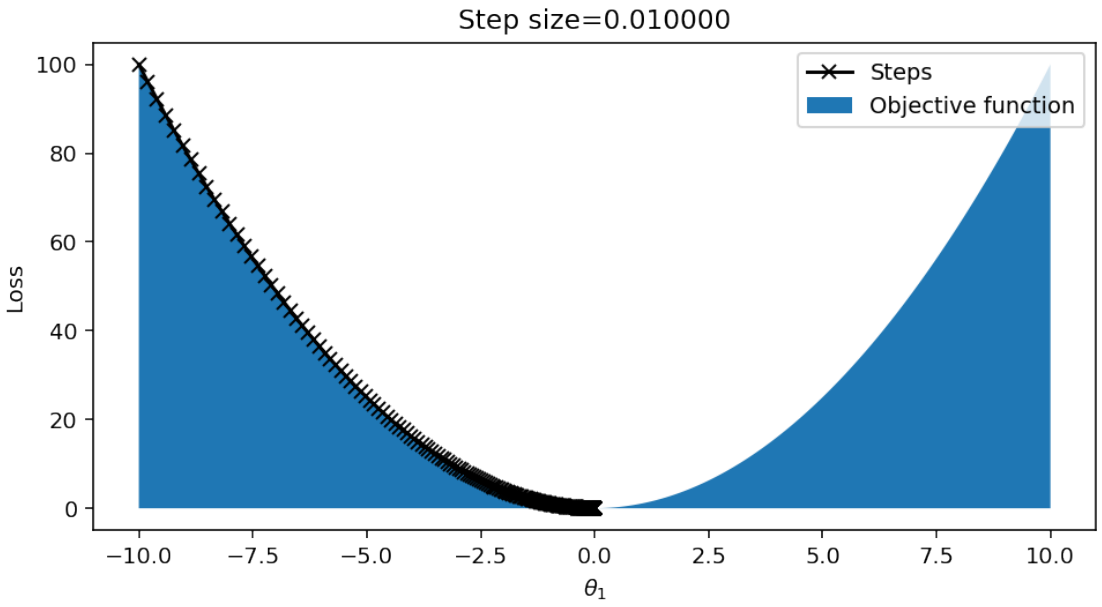


6.6.1 Why step size matters

The step size δ is critical for success. If it is too small, the steps will be very small and convergence will be slow. If the steps are too large, the behaviour of the optimisation can become quite unpredictable. This happens if the gradient functions changes significantly over the space of a step (e.g. if the gradient changes sign across the step).

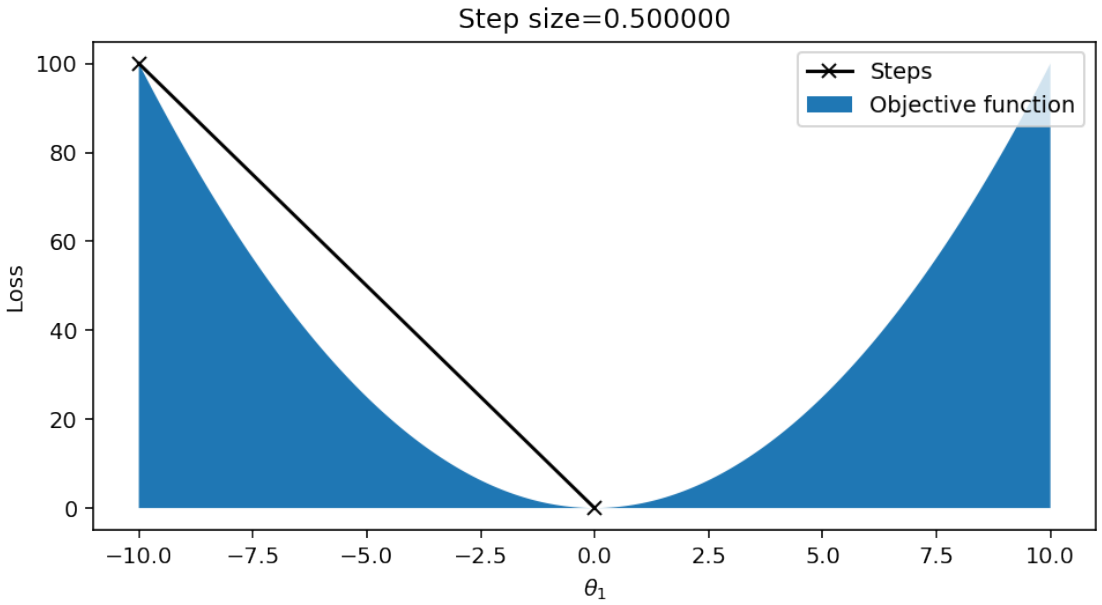
[27]:
```
## too slow
# step = 0.01
plot_gradient_descent(xs, L, dL, [-10.], 0.01)
```

```
Converged in 606 steps
```



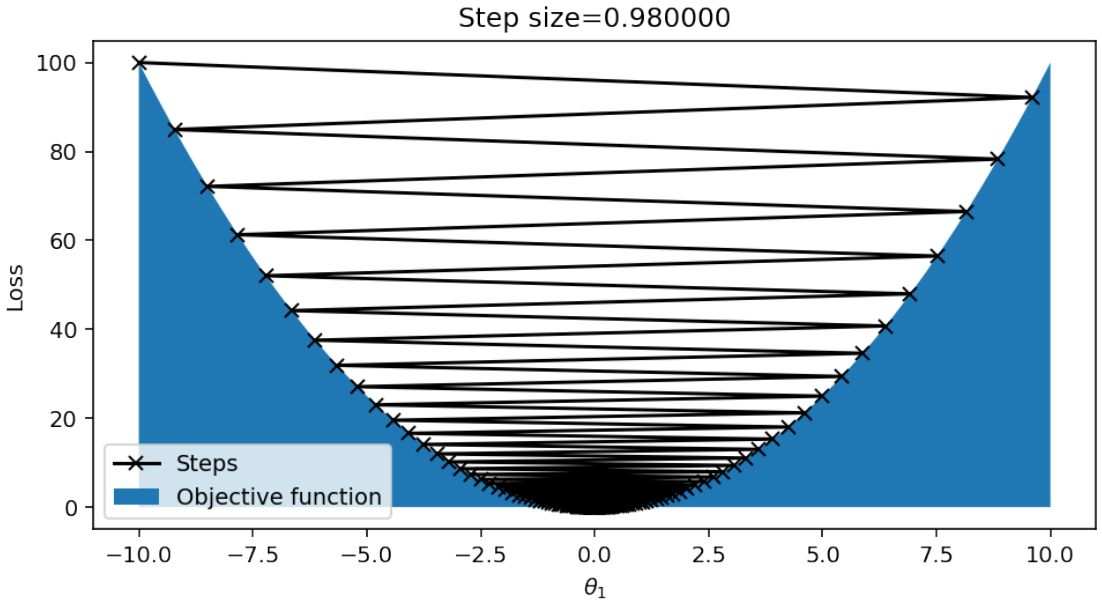
[28]:
```
# perfect :)
# step = 0.5
plot_gradient_descent(xs, L, dL, [-10.], 0.5)
```

```
Converged in 2 steps
```



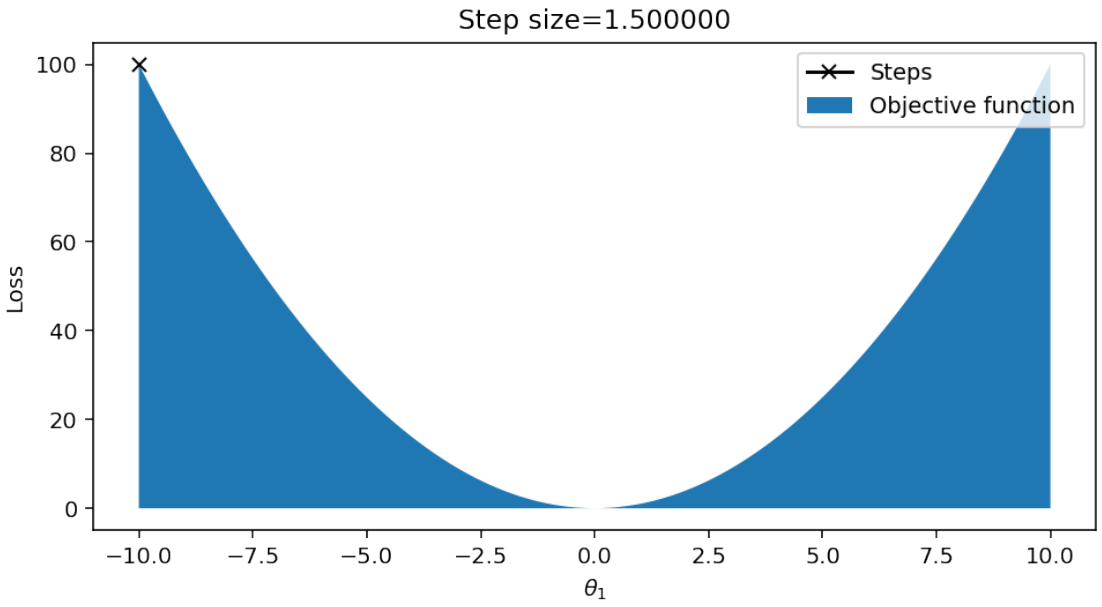
[29]:
```
# too fast -- oscillation occurs
plot_gradient_descent(xs, L, dL, [-10.], 0.98)
```

```
Converged in 301 steps
```



[30]:
```
# way too fast -- diverges
plot_gradient_descent(xs, L, dL,
                      [-10.], 1.5)
```

```
Converged in 1023 steps

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
overflow encountered in square

C:\Users\John\Dropbox\teaching\df3-2020\lectures\week_7_optimisation_II\utils\hi
story.py:81: RuntimeWarning: invalid value encountered in subtract
  self.loss_change = self.last_loss - loss
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning:
overflow encountered in multiply

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:26: RuntimeWarning:
invalid value encountered in add
C:\Users\John\Dropbox\teaching\df3-2020\lectures\week_7_optimisation_II\utils\hi
story.py:85: RuntimeWarning: invalid value encountered in less
  if loss<self.best or force:
```



6.6.2 Relationship to Lipschitz constant

We won't show this, but the optimal step size δ is directly related to the Lipschitz constant K of the objective function. Unfortunately we rarely know K precisely in many real-world optimisation tasks, and step size is often set by approximate methods like line search.

6.6.3 Gradient descent in 2D

This technique extends to any number of dimensions, as long as we can get the gradient vector at any point in the parameter space. We just have a gradient vector $\nabla L(\theta)$ instead of a simple 1D derivative. There is no change to the code.

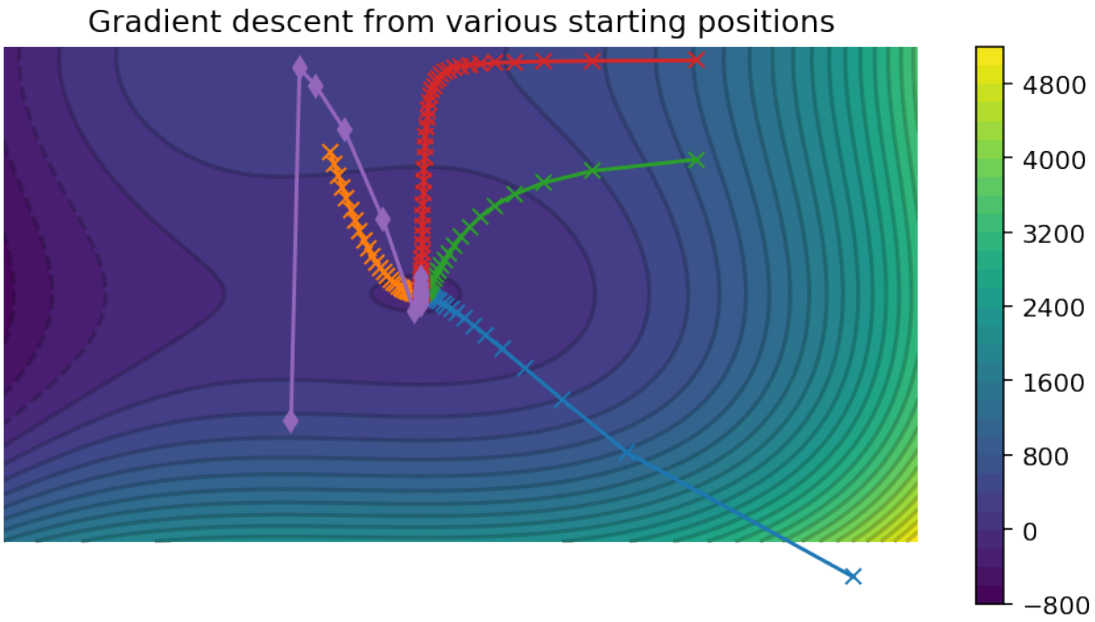
[32]:
```
# test gradient descent in 2D
# you don't need to understand this code

### create a test function
from numpy.polynomial import polynomial

# a compact way of writing
# y^2 - 0.02y^3 + 5x + x^2 + 0.04x^3
poly = np.array([[0,0,1,-0.02],
                 [5,0,0,0],
                 [1,0,0,0],
                 [0.04,0,0,0]])

# we can take the derivative exactly,
# since polynomial functions have known analytic derivative
```

```
# this function does this for us --
# it is a very simple array operation
der_x, der_y = (polynomial.polyder(poly, axis=0),
                polynomial.polyder(poly, axis=1))

# loss
def L(x):
    return polynomial.polyval2d(x[0], x[1], poly)

# note that the gradient has two components,
# because its a 2D function
def dL(x):
    return np.array([polynomial.polyval2d(x[0], x[1], der_x),
                     polynomial.polyval2d(x[0], x[1], der_y)])
```

[33]:
```
# plot the surface
div = np.linspace(-35,35,100)
mx, my = np.meshgrid(div, div)
mz = L([mx, my])

fig = plt.figure()
ax = fig.add_subplot(1,1,1)
contour = ax.contourf(mx, my, mz, 32)
ax.contour(mx, my, mz, 30, colors='k', alpha=0.2)


# now plot some optimisation histories
# using gradient descent
# all of them with the same fixed size
res = gradient_descent(L, dL, [30.0,-40.0], 0.1, tol=1e-6)
history = res.best_thetas

ax.plot(history[:,0], history[:,1], 'C0-x')

res = gradient_descent(L, dL, [-10.0,20.0], 0.1, tol=1e-6)
history = res.best_thetas
ax.plot(history[:,0], history[:,1], 'C1-x')

res = gradient_descent(L, dL, [18.0,19.0], 0.1, tol=1e-6)
history = res.best_thetas
ax.plot(history[:,0], history[:,1], 'C2-x')

res = gradient_descent(L, dL, [18.0,33.0], 0.1, tol=1e-6)
history = res.best_thetas
ax.plot(history[:,0], history[:,1], 'C3-x')
```

```
res = gradient_descent(L, dL, [-13.0,-18.0], 0.9, tol=1e-6)
history = res.best_thetas
ax.plot(history[:,0], history[:,1], 'C4-d')
ax.axis("off")
ax.set_title("Gradient descent from various starting positions")
fig.colorbar(contour)
```

[33]: <matplotlib.colorbar.Colorbar at 0x1fb381ac588>



6.7 Gradients of the objective function

For first-order optimisation to be possible, the derivative of the objective function has to be available. This obviously does not apply directly to empirical optimisation (e.g. real world manufacturing where the quality of components is being tested in an experiment – there are no derivatives), but it can be applied in many cases where we have a computational model that can be optimised. This is again a reason to favour building models when optimising.

6.7.1 Why not use numerical differences?

The definition of differentiation of a function $f(x)$ is the well known formula:

$$\frac{d}{dx}f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h}$$

Given this definition, why do we need to know the *true derivative* $\nabla L(\theta)$ if we can evaluate $L(\theta)$ anywhere? Why not just evaluate $L(\theta + h)$ and $L(\theta - h)$ for some small h? This approach is called numerical differentiation, and these are **finite differences**.

This works fine for reasonably smooth one-dimensional functions:

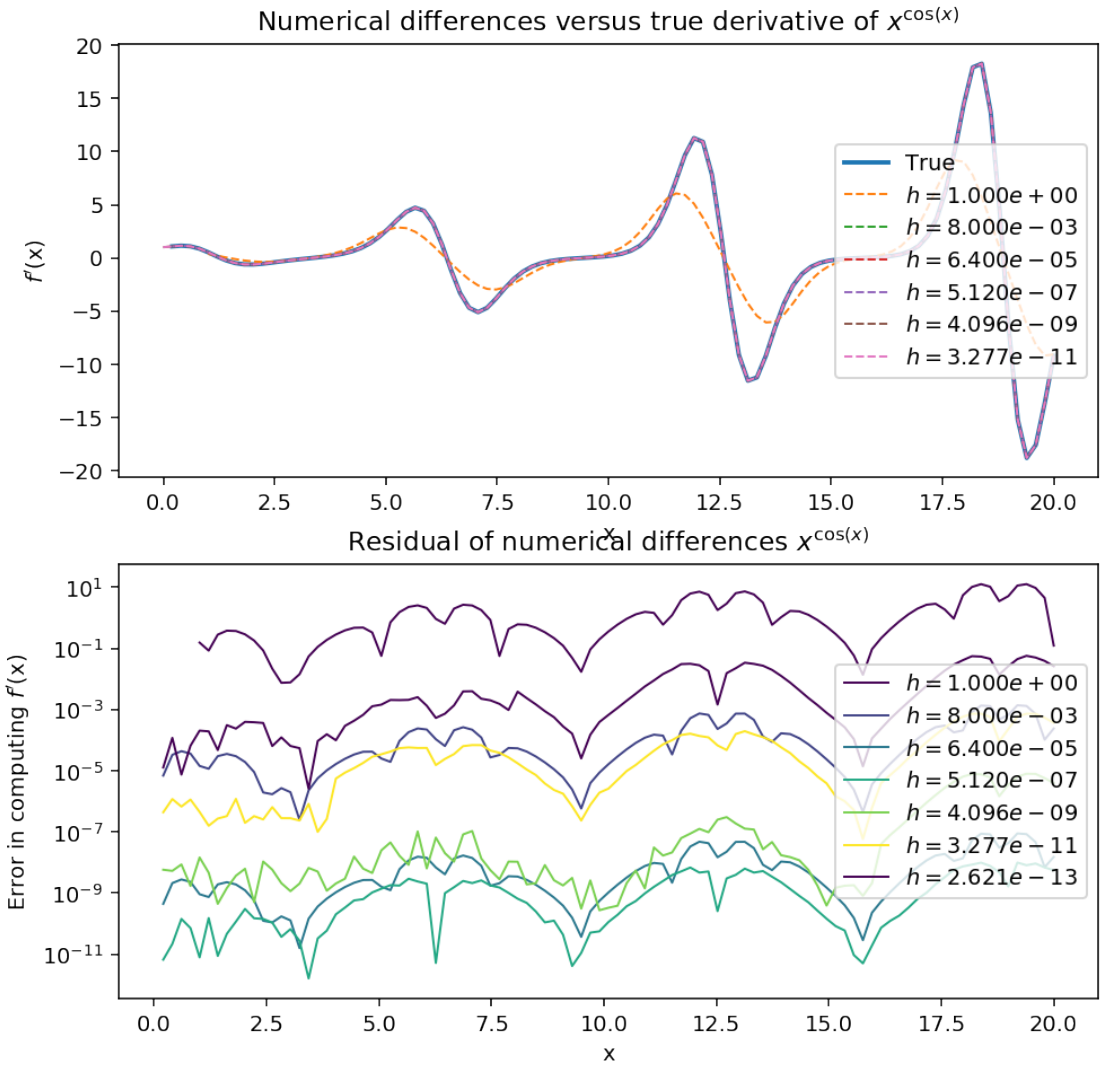
[34]:
```
def f(x):
    return x**(np.cos(x))

def df(x): # true, exact derivative
    return x**(np.cos(x)-1) * (np.cos(x)-x*np.log(x)*np.sin(x))

# finite differences
def approx_d(f, x, delta=1e-4):
    return (f(x+delta) - f(x-delta)) / (2*delta)


# plot the results over the range -10, 10
fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(2,1,1)
x = np.linspace(0,20, 100)

plt.rcParams["axes.prop_cycle"] = plt.cycler("color", plt.cm.viridis(np.
 ↪linspace(0,1,6)))



## Plot the derivative and its approximate form
ax.plot(x,df(x), label="True",lw=2)
for d in range(0,18,3):
    ax.plot(x,approx_d(f, x, delta=5**-d), ls='--', lw=1, label="$h=%.
 ↪3e$"%(5**-d))

ax.legend(loc='right')
ax.set_title("Numerical differences versus true derivative of $x^{\cos(x)}$")
ax.set_xlabel("x")
ax.set_ylabel("$f^\\prime$(x)")

## Plot the residuals
ax = fig.add_subplot(2,1,2)


for d in range(0,20,3):
    # adjust to 20 to see numerical issues
    d = d
    ax.plot(x,np.abs(df(x)-approx_d(f, x, delta=5**-d)), ls='-', lw=1,␣
 ↪label="$h=%.3e$"%(5**-d))

ax.set_yscale("log")
ax.legend(loc='right')
ax.set_title("Residual of numerical differences $x^{\cos(x)}$")
```

```python
ax.set_xlabel("x")
ax.set_ylabel("Error in computing $f^\\prime$(x)")
```

```
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power
```

```
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning:
invalid value encountered in power

c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
divide by zero encountered in log
  """
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:5: RuntimeWarning:
invalid value encountered in multiply
  """
```

```
[34]: Text(0, 0.5, 'Error in computing $f^\\prime$(x)')
```



6.7.2 Numerical problems

It is also difficult to choose h such that the function is not misrepresented by an excessive value but numerical issues do not dominate the result. Remember that finite differences violates *all* of the rules for good floating point results:

$$\frac{f(x+h) - f(x-h)}{2h}$$

- (a) it adds a small number h to a potentially much larger number x *(magnitude error)*
- (b) it then subtracts two very similar numbers $f(x+h)$ and $f(x-h)$ *(cancellation error)*
- (c) then it divides the result by a very small number $2h$ *(division magnification)*

It would be hard to think of a simple example that has more potential numerical problems than finite differences!

6.7.3 Revenge of the curse of dimensionality

This is not useful in high dimensions, even if we can deal with numerical issues, however. The **curse of dimensionality** strikes once again. To evaluate the *gradient* at a point $\vec{x}$ we need to compute the numerical differences in *each* dimension x_i. If $\vec{\theta}$ has one million dimensions, then *each* individual derivative evaluation will require two million evaluations of $L(\theta)$! This is a completely unreasonable overhead. The acceleration of first-order methods over zeroth-order would be drowned out by the evaluation of the gradient.

7 Improving gradient descent

Gradient descent can be very efficient, and often **much** better than zeroth-order methods. However, it has drawbacks:

- The gradient of the loss function $L'(\theta) = \nabla L(\theta)$ must be computable at any point θ. **Automatic differentation** helps with this.
- Gradient descent can get stuck in local minima. This is an inherent aspect of gradient descent methods, which will not find global minima except when the the function is convex *and* the step size is optimal. **Random restart** and **momentum** are approachs to reduce sensitivity to local minima.
- Gradient descent only works on smooth, differentiable objective functions. **Stochastic relaxation** introduces randomness to allow very steep functions to be optimised.
- Gradient descent can be very slow if the objective function (and/or the gradient) is slow to evaluate. **Stochastic gradient descent** can massively accelerate optimisation if the objective function can be written as a simple sum of many subproblems.

7.1 Automatic differentiation

This problem can be solved if we know analytically the derivative of the objective function in closed form. For example, the derivative of the least squares linear regression that we saw in the last lecture is (relatively) easy to work out exactly as a formula. However, it seems very constraining to have to manually work out the derivative of the objective function, which might be very complicated indeed for a complex multidimensional problem. This is the major motivation for **algorithmic differentiation** (or **automatic differentiation**).

Automatic differentiation can take a function, usually written a *subset* of a full programming language, and automatically construct a function that evaluates the exact derivative at any given point. This makes it feasible to perform first-order optimisation.

7.2 Programming language advances

In DF(H) we will see three major advances in *programming* that power data science.

- **Vectorised programming**
  - *Example:* NumPy, eigen, nd4j, J
  - Provides native operations over tensors, potentially with GPU acceleration.
- **Differentiable programming**
  - *Examples:* autograd, JAX, pytorch, tensorflow

  - Automatically differentiates vectorised code, producing exact derivatives of tensor algorithms.
- **Probabilistic programming**
  - *Examples:* pymc, stan, edward, Uber, Pyro, webppl
  - Allows values to be uncertain, with (tensor, differentiable) random variables as first class values.

Each of these advances provides a massive leap in the expressive power of the language and makes it possible to elegantly and compactly work with algorithms which would otherwise be tedious and arcane.

7.2.1 The magic behind modern advances in data science

Some of the most common implementations of this technique are in deep learning software packages like *TensorFlow*, *Theano*, *Torch/PyTorch*. These provide a way of defining a **computational graph** (implictly or explicitly) which defines the operations to be performed, and from which the corresponding derivative computation can be derived. These implementations tend to be focused on the operations used in neural networks, like matrix multiplication and elementwise nonlinear functions, and they tend not to include branching or iteration (or support very limited forms of conditional/looping expressions).

7.2.2 Autograd

Other software, like autograd provides automatic differentiation for virtually any NumPy code. The example below is from the autograd documentation. It is a drop in replacement which just "magically" estimates derivatives (although only some operations are supported).

autograd has now evolved into **Google JAX**, probably the most promising machine learning library. JAX supports GPU and TPU computation with automatic differentation. I'm not using it here because it is hard to install.

[ ]:
```
# uncomment if you want to install this
# !pip install git+git://github.com/HIPS/autograd
```

[35]:
```
# code from: https://github.com/HIPS/autograd
# MIT License: see https://github.com/HIPS/autograd/blob/master/license.txt
# note: you will need to install autograd to get this to work!

import autograd.numpy as np
from autograd import grad, elementwise_grad

# just plain numpy
def tanh(x):  # Define a function
    y = np.exp(-x)
    return (1.0 - y) / (1.0 + y)


# compute gradient
grad_tanh = grad(tanh)  # Obtain its gradient function
```

```
print(grad_tanh(1.0))  # Evaluate the gradient at x = 1.0
```

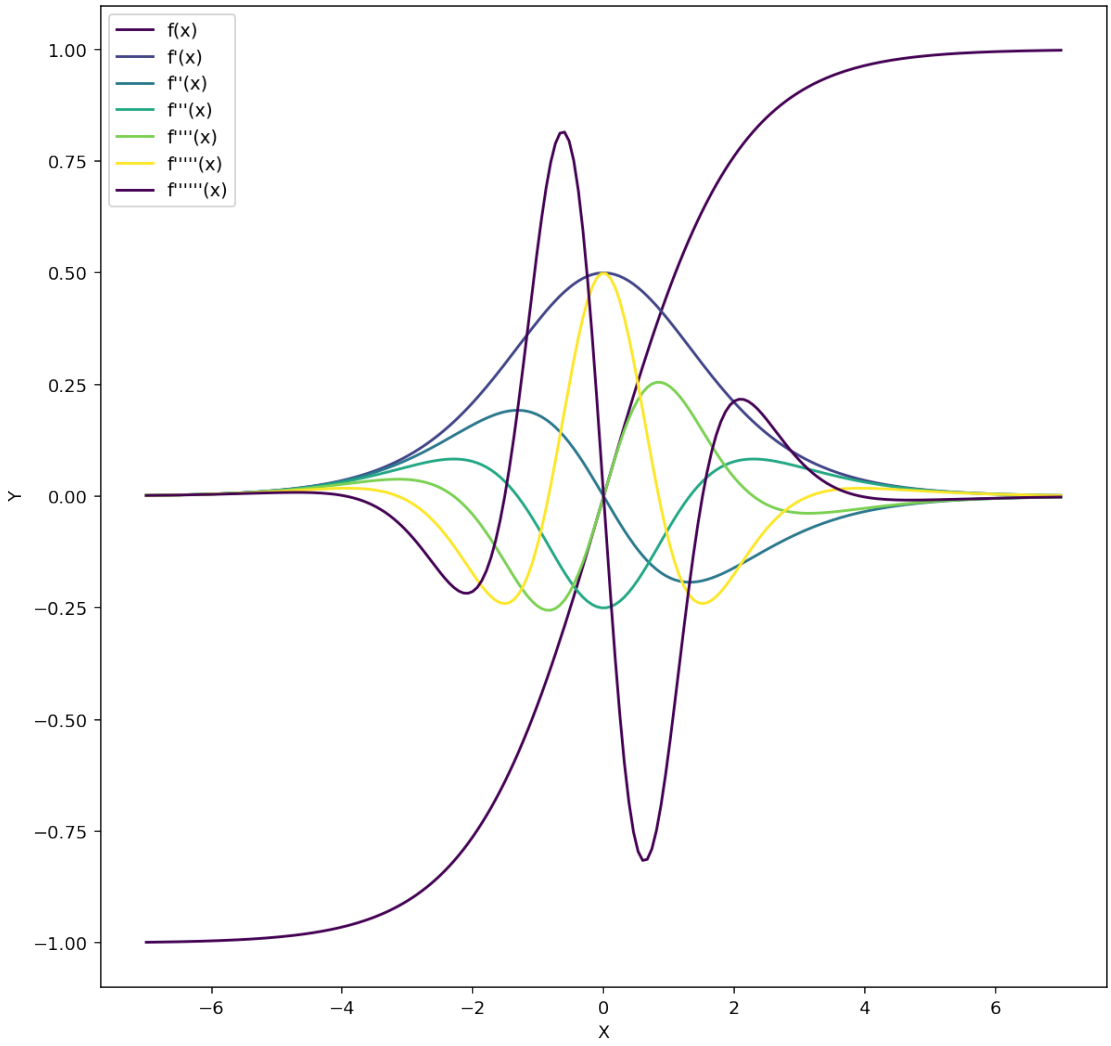
```
0.39322386648296376
```

[36]:
```
# Compare to finite differences
print((tanh(1.0001) - tanh(0.9999)) / 0.0002)
```

```
0.39322386636453377
```

[37]:
```
x = np.linspace(-7, 7, 200)
gr = elementwise_grad
fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(1,1,1)
ax.plot(x, tanh(x),
          x, gr(tanh)(x),                                  # first  derivative
          x, gr(gr(tanh))(x),                             # second derivative
          x, gr(gr(gr(tanh)))(x),                        # third  derivative
          x, gr(gr(gr(gr(tanh))))(x),                   # fourth derivative
          x, gr(gr(gr(gr(gr(tanh)))))(x),              # fifth  derivative
          x, gr(gr(gr(gr(gr(gr(tanh))))))(x))  # sixth  derivative

ax.set_xlabel("X")
ax.set_ylabel("Y")
ax.legend(["f(x)", "f'(x)","f''(x)", "f'''(x)", "f''''(x)", "f'''''(x)",␣
 ↪"f''''''(x)"])
```

[37]:
```
<matplotlib.legend.Legend at 0x1fb387074e0>
```



[39]:
```
# vector -> scalar runction

def tanh_sum_sqr(x, k):  # Define a function
    return np.tanh(np.sum(x**2)-k)

tanh_sum_sqr(np.array([-0.1, 0.2, 0.6]), 0.5)
```

[39]:
```
-0.08975778474716013
```

[40]:
```
grad_t_s_s = grad(tanh_sum_sqr) # function -> function

# differentiates w/respect to first arg. only
grad_t_s_s(np.array([-0.1, 0.2, 0.3]), 0.5)
```

[40]:
```
array([-0.17616545,  0.35233091,  0.52849636])
```

7.2.3 Vectorised example

[41]:
```
# I do not fancy trying to differentiate this by hand
# (actually it's not that hard)
# (just really annoying)
f = np.array([[1, -0.2], [0.8, 1.5]])


def dog(x):
    x = x @ f
    return np.exp(-np.sum(x ** 2, axis=1) / 10.0) - np.exp(
        -np.sum(x ** 2, axis=1) / 2.0
    )


ddog = elementwise_grad(dog)  # compute derivative via autograd
# that is *literally* all that is required
```

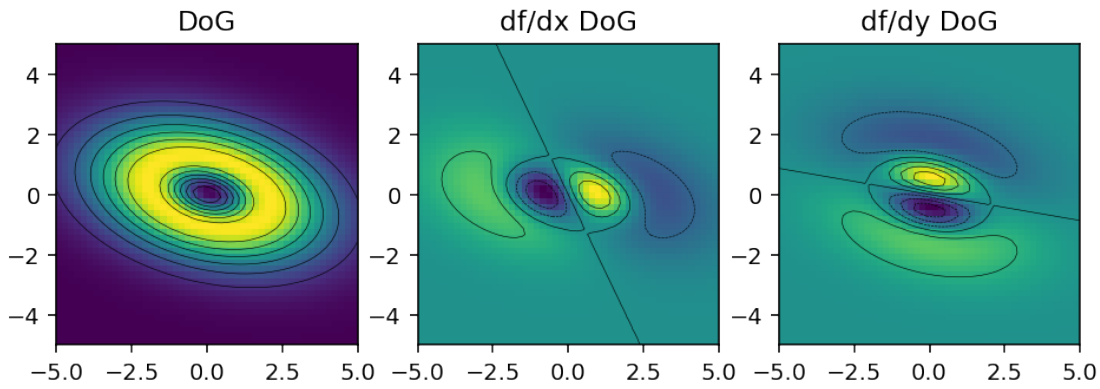
[42]:
```
## plot the results
# generate a grid to evaluate the function over
def show_fn(ax, fn, r, n_steps, d=None, contours=20):
    spacing = np.linspace(r[0], r[1], n_steps)
    mx, my = np.meshgrid(spacing, spacing)

    # rearrange the points into a Nx2 array
    pts = np.stack([mx.ravel(), my.ravel()]).T
    if d is None:
        mz = fn(pts).reshape(mx.shape)
    else:
        mz = fn(pts)[:, d].reshape(mx.shape)
    ax.pcolor(mx, my, mz)
    ax.contour(mx, my, mz, colors="k", linewidths=0.3, contours=contours)
    ax.set_aspect(1.0)
```

[43]:
```
## plot the results
# generate a grid to evaluate the function over

# plot the results
fig = plt.figure()
ax = fig.add_subplot(1, 3, 1)
show_fn(ax, dog, [-5, 5], 50)
ax.set_title("DoG")
ax = fig.add_subplot(1, 3, 2)
show_fn(ax, ddog, [-5, 5], 50, d=0)
ax.set_title("df/dx DoG")
ax = fig.add_subplot(1, 3, 3)
show_fn(ax, ddog, [-5, 5], 50, d=1)
```

```
ax.set_title("df/dy DoG")
```

```
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:14: UserWarning: The
following kwargs were not used by contour: 'contours'
```

[43]: `Text(0.5, 1.0, 'df/dy DoG')`



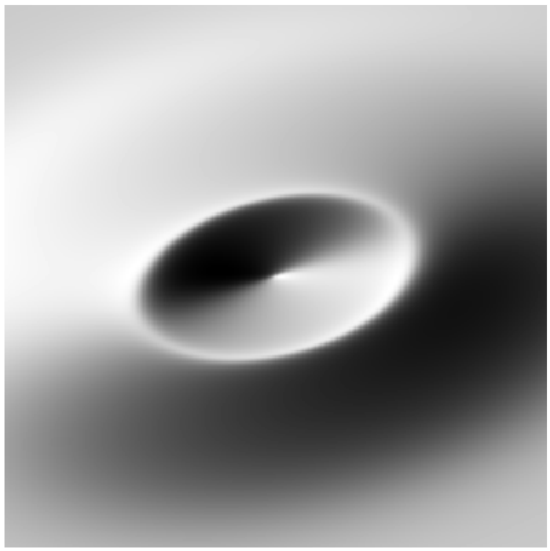
7.3 Derivative tricks

[*Side note: if you have the gradient of a function, you can do nifty things like computing the light that would be reflected from the surface, given a fixed light source. This isn't directly important for DF(H), but shows how useful being able to differentiate functions is*]

[44]:
```
# You can ignore this if you want
# it just shows how the derivative can be useful
# in visualising a function, by computing lighting
# effects
fig = plt.figure()
ax = fig.add_subplot(1, 2, 1)
spacing = np.linspace(-4, 4, 300)
mx, my = np.meshgrid(spacing, spacing)
# rearrange the points into a Nx2 array
pts = np.stack([mx.ravel(), my.ravel()]).T

# stack up the gradient vectors
dzdx = ddog(pts)[:, 0]
dzdy = ddog(pts)[:, 1]
dzdz = np.ones_like(dzdy) * 0.08

grad_vec = np.stack([dzdx, dzdy, dzdz]).T
# normalise gradient vector
grad_vec = (grad_vec.T / (np.linalg.norm(grad_vec, axis=1))).T
```

```
# compute dot product with light vecotr
light_vec = np.array([0.5, 0.3, 0.5])
light = np.sum(grad_vec * light_vec / np.linalg.norm(light_vec), axis=1)

ax.imshow(light.reshape(mx.shape), cmap="gray")
ax.axis("off")
```

[44]: (-0.5, 299.5, 299.5, -0.5)



7.4 Using autograd in optimisation

Using automatic differentiation, we can write down the form of the objective function as a straightforward computation, and get the derivatives of the function "for free". This makes it extremely efficient to perform first-order optimisation.

This is what machine learning libraries do. They just make it easy to write vectorised, differentiable code that runs on GPU/TPU hardware. The rest is just dressing.

7.4.1 Fitting a line, first-order

Let's re-solve the line of best fit from lecture 6. We want to find m and c; the parameters of a line, such that the square difference between the line and a set of datapoints is minimised (the objective function).

[46]:
```
## generate some random data, with a linear trend
# the linear regression problem; find m and c in the equation y=mx+c
from utils.history import linear_regression_plot

line_x = np.sort(np.random.normal(0, 1, (20,)))
```

```
gradient, offset = 2, 1  # these are the "true" parameters that generated this␣
 ↪data

# 2x + 1 and a bit of noise
line_y = (
    gradient * line_x + offset + np.random.normal(0, 0.5 * np.abs(line_x),␣
 ↪line_x.shape)
)

# loss function
def loss(theta):
    # sum of squares
    e = np.sum(((line_x * theta[0] + theta[1]) -
                line_y) ** 2)
    return e
```

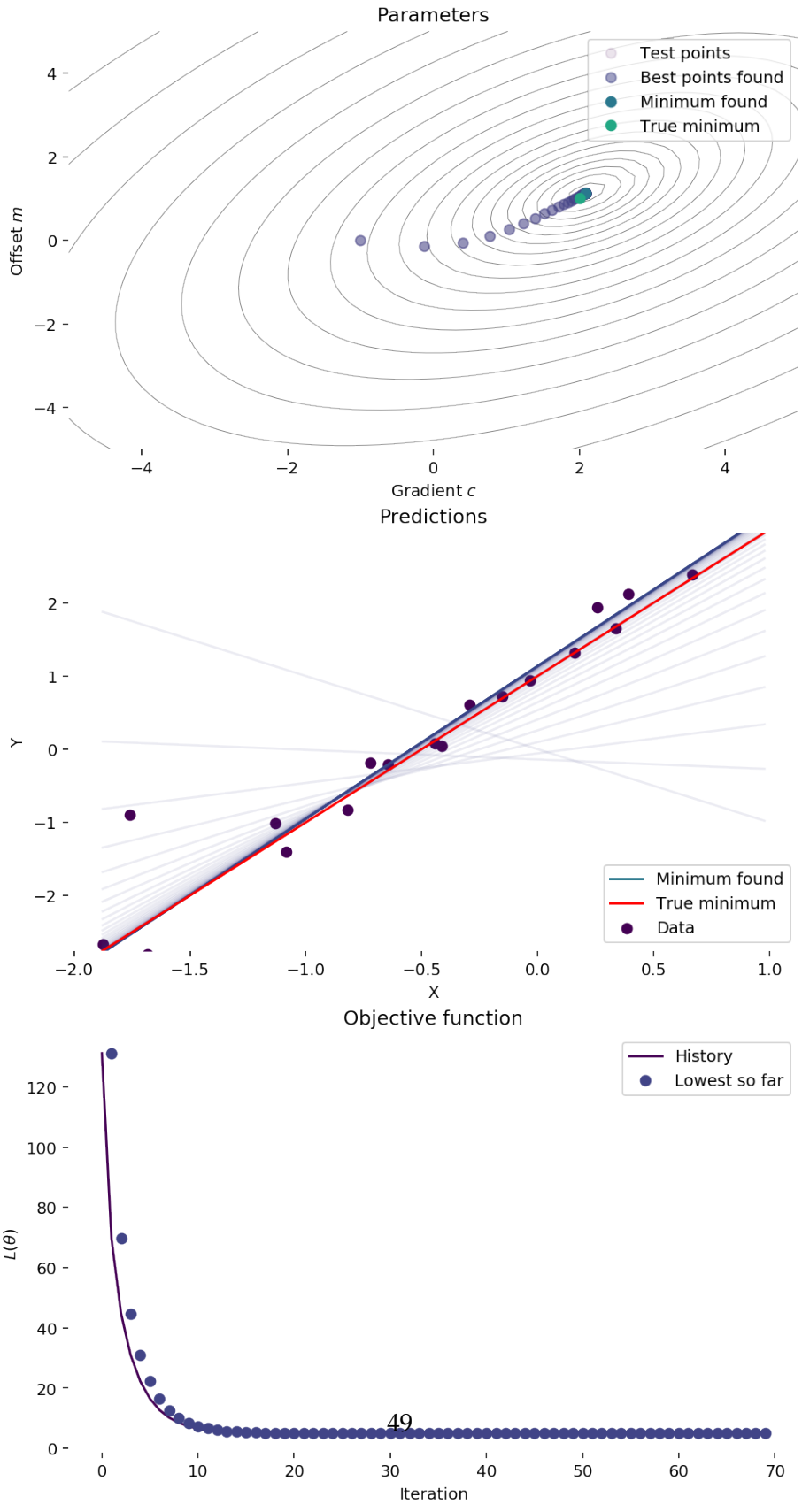
Here's the special bit:

[47]:
```
#### new stuff
# compute derivative (in one step!)
dloss = grad(loss)


# optimise with gradient descent
grad_results = gradient_descent(loss, dloss,
                                np.array([-1.0,0.0]),
                                0.01)
print(grad_results.iters)
```

```
69
```

[48]:
```
linear_regression_plot(grad_results, gradient, offset, line_x,
                       line_y, opt_title="Gradient descent")
```

Gradient descent over possible line configurations



7.5 Limits of automatic differentiation

Obviously, differentiation is only available for functions that are differentiable. While first-order gradient vectors are often computable in reasonable time, as we'll see later it becomes very difficult to compute second derivatives of multidimensional functions.

7.5.1 Stochastic relaxation

How do animals evolve camouflage? This question is posed and discussed in **"The Blind Watchmaker"** by *Richard Dawkins*. Evolution is a gradual optimisation process, and to make steps that might be accepted requires that there is a smooth path from "poor fitness" to "good fitness".

.Image by dano272 shared CC BY-ND

So how can an animal like a moth evolve camouflage? It either gets eaten by a predator who sees it or the predator does not see it. This is binary function and has no gradient. While evolution requires no gradient, it does require that there be approximately continuous fitness functions.

7.5.2 Resolution

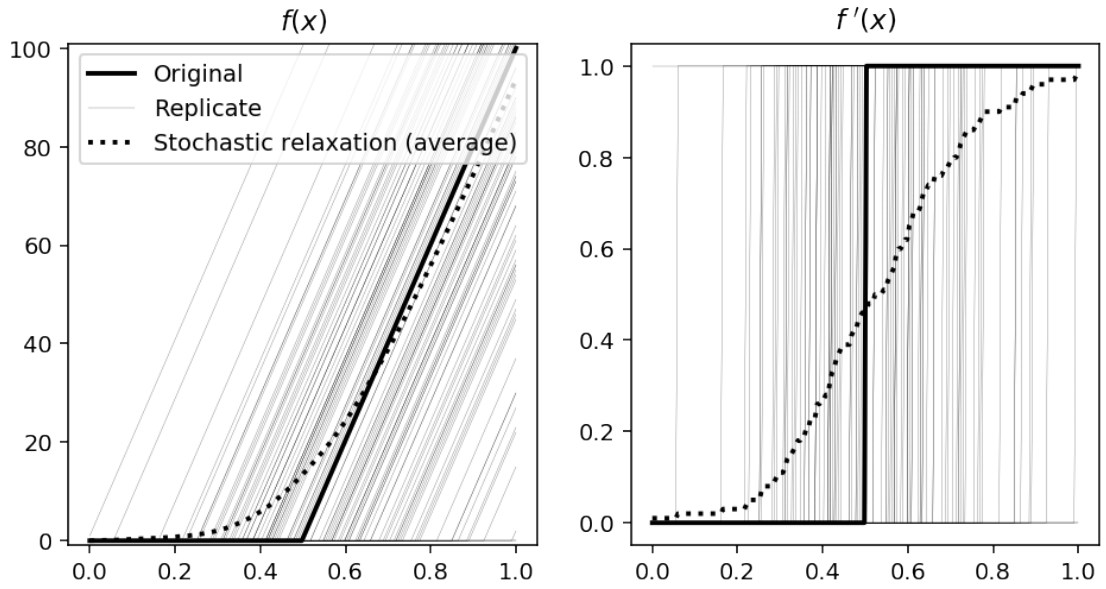
The argument is that although every *specific* case is a simple binary choice, it is *averaged* over many random instances, where the conditions will be slightly different (maybe it is nearly dark, maybe the predator has bad eyes, maybe the weather is foggy) and averaging over all of those cases, some very minor change in colouring might offer an advantage. Mathematically speaking, this is **stochastic relaxation**; the apparently impossibly steep gradient has been rendered (approximately) Lipschitz continuous by integrating over many different random conditions.

This is applicable to many problems outside of evolution. For example, a very steep function has a very large derivative at some point; or it might have zero derivative in parts. But if we average over lots of cases where the step position is very slightly shifted, we get a smooth function.

[49]:
```
fig = plt.figure()
f_ax = fig.add_subplot(1,2,1)
d_ax = fig.add_subplot(1,2,2)

# hard step function
def step(x,t):
    return np.where(x>t, 1, 0)

xs = np.linspace(0,1,200)
fn = step(xs, 0.5)
f_ax.plot(xs, np.cumsum(fn), 'k', lw=2, label="Original")
d_ax.plot(xs, fn, 'k', lw=2, label="Original")
f_ax.set_title("$f(x)$")
d_ax.set_title("$f^{\ \prime}(x)$")
```

```
# but if we average it with slight shifts
# we get a function that is smoother
# we don't know the derivative exactly
# but that, it turns out, doesn't matter...
average_step = np.zeros_like(xs)
for i in range(100):
    offset = np.random.normal(0,0.2)
    rnd_step = step(xs, 0.5+offset)
    f_ax.plot(xs, np.cumsum(rnd_step), lw=0.1, c='k')
    d_ax.plot(xs, rnd_step, lw=0.1, c='k')
    average_step += rnd_step
f_ax.plot(xs, np.cumsum(rnd_step), lw=0.1, c='k', label="Replicate")
d_ax.plot(xs, rnd_step, lw=0.1, c='k', label="Replicate")
f_ax.set_ylim(-1,101)
d_ax.plot(xs, average_step/100.0, 'k:', lw=2, label="Stochastic relaxation␣
 ↪(average)")
f_ax.plot(xs, np.cumsum(average_step)/100.0, 'k:', lw=2, label="Stochastic␣
 ↪relaxation (average)")
f_ax.legend(loc='upper center')
```

[49]: <matplotlib.legend.Legend at 0x1fb3a60d710>



7.6 Stochastic gradient descent

Gradient descent evaluates the objective function and its gradient at each iteration before making a step. This can be very expensive to do, particularly when optimising function approximations with large data sets (e.g. in machine learning).

If the objective function can be broken down into small parts, the optimiser can do gradient descent on randomly selected parts independently, which may be much faster. This is called **stochastic gradient descent (SGD)**, because the steps it takes depend on the random selection of the parts of the objective function.

This works if the objective function can be written as a sum:

$$L(\theta) = \sum_i L_i(\theta),$$

i.e. that the objective function is composed of the sum of many simple sub-objective functions $L_1(\theta), L_2(\theta), \ldots, L_n(\theta)$.

This type of form often occurs when matching parameters to observations – **approximation problems**, as in machine learning applications. In these cases, we have many **training examples** $\vec{x}_i$ with matching known outputs y_i, and we want find a parameter vector θ such that:

$$L(\theta) = \sum_i ||f(\vec{x}_i; \vec{\theta}) - y_i||$$

is minimised, i.e. that the difference between the model output and the expected output is minimised, *summing over all training examples*.

Differentiation is a linear operator. This means that we can interchange summation, scalar multiplication and differentiation $\frac{d}{dx}(af(x) + bg(x)) = a\frac{d}{dx}f(x) + b\frac{d}{dx}g(x)$, we have:

$$\nabla \sum_i ||f(\vec{x}_i; \vec{\theta}) - y_i|| = \sum_i \nabla ||f(\vec{x}_i; \vec{\theta}) - y_i||$$

In this case, we can take any *subset* of training samples and outputs, compute the gradient for each sample, then make a move according to the computed gradient of the subset. Over time, the random subset selection will (hopefully) average out. Each subset is called a **minibatch** and one run through the whole dataset (i.e. enough minibatches so that every data item has been "seen" by the optimiser) is called an **epoch**.

7.6.1 Memory advantages

SGD has major advantages in terms of memory consumption, because computations can be applied to a small number of samples in **minibatches**. We just compute the gradient on a subsample, and move in that direction. It won't be *exactly* the right derivative of the whole objective function, but it will be a good approximation.

Particularly on memory-constrained devices such as GPUs (which might have only 12-16GB of RAM even for powerful GPUs), it can be impossible to store the entire dataset on the device. Splitting up into batches can get around this limitation. It can also have advantages with respect to the *memory hierarchy* – small batches of data may induce fewer cache misses and thus result in enhanced performance.

7.6.2 Heuristic enhancement

As well as plain memory efficiency, SGD can actually improve the performance of optimisation in terms of the objective function decrease, particularly by reducing the likelihood of getting stuck in minima. This is because the random partitioning of the objective function in each minibatch adds *noise* to the optimisation process. This might at first seem like a problem; we don't want the optimisation to be inaccurate. But noise means that there is a chance that gradient descent will *not* go downhill, but instead might go up hill and jump over a maxima.

While adding noise is a **heuristic search** approach (there is no guarantee it will make things better or even not make things worse), it is often very effective. We are essentially getting the benefits of a limited form of **stochastic relaxation** – our objective function can be "smoothed out" by averaging over random subsamples, so even if it is not quite Lipschitz continuous (or has a bad Lipschitz constant), SGD can work well.

7.6.3 Using SGD

There is no guarantee that SGD will even move in the right direction. In practice, it can be very efficient for many real world problems. For example, let's consider again the problem of fitting a line to observations (**linear regression**).

Given a set of pairs x_i, y_i, we want to find parameters $\vec{\theta} = [m, c]$ that minimise the squared error between the function $y' = f(x; m, c) = mx + c$ and the true known output y. The objective function is:

$$\begin{aligned} &\sum_i ||f(\vec{x}_i; \vec{\theta}) - y_i||_2^2 \\ =&\sum_i ||(mx_i + c) - y_i||_2^2 \end{aligned}$$

Rather than computing the whole sum, we can compute the gradient on a **random** subset, and use this to compute the next step.

[50]:
```
import autograd.numpy as np
def sgd(L, dL, theta_0, xs, ys, step=0.1, batch_size=10, epochs=10):
    """L: Objective function, in the form L(theta, xs, ys)
       dL: derivative of objective function in form dL(theta, xs, ys)
       theta_0: starting guess
       xs: vector of inputs
       ys: vector of outputs
       step: step size
       batch_size: batchsize
    """
    theta = np.array(theta_0)
    grad = np.zeros_like(theta_0)

    o = History()

    # One epoch is one run through the whole dataset
```

```
    for epoch in range(epochs):
        batch = np.arange(len(xs))
        # randomize order
        np.random.shuffle(batch)
        subset_index = 0
        # iterate over subsets

        ## One batch
        while subset_index + batch_size <= len(xs):

            # accumulate partial gradient
            i,j = subset_index, subset_index+batch_size

            # compute gradient on the random subset
            # accumulating the gradient direction as we go
            grad = dL(theta, xs[batch[i:j]], ys[batch[i:j]])  / (j-i)
            # next batch please!
            subset_index += batch_size

            # make a step
            theta = theta - grad * step
            o.track(theta, L(theta, xs, ys))

        #o.track(theta, L(theta, xs, ys))
    return o.finalise()
```

7.6.4 Linear regression with SGD

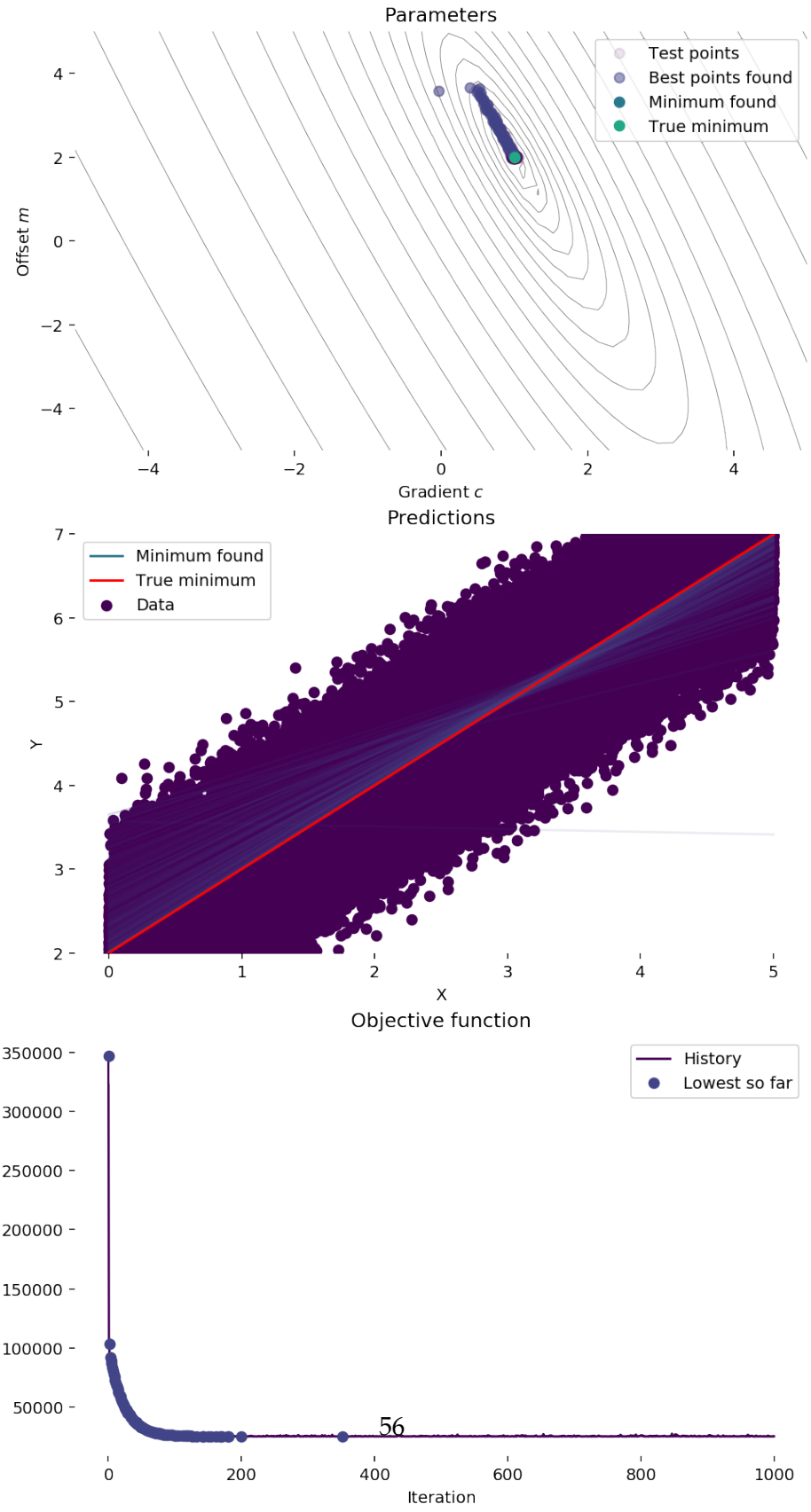
We can do our linear regression example with 10000 points - and find a good fit with *only one pass through the data*. This works because we can divide the problem up into a lots of sums of smaller problems (fitting a line on a few random points at a time) which are all part of one big problem (fitting a line to all of the points).

When this is possible, it is vastly more efficient than computing the gradient for the entire set of data we have available.

[51]:
```
# 100000 data points
xs = np.linspace(0,5, 100_000)
ys = xs  * 1.0 + 2.0
ys = ys + np.random.normal(0,0.5,xs.shape)

def linear_loss(theta,xs,ys):
    y_prime = theta[0] * xs + theta[1]
    loss = np.sum((y_prime-ys)**2)
    return loss

def linear_dloss(theta,xs,ys):
    return grad(lambda x:linear_loss(x,xs,ys))(theta)
```

[52]:
```
res = sgd(linear_loss, grad(linear_loss), [-3.5, 2.5], xs, ys,
          batch_size=100, epochs=1, step=0.05)

linear_regression_plot(res, 1.0, 2.0, xs, ys, 'SGD')
```

SGD over possible line configurations



7.7 A nightmare function

This function has it all: * narrow valleys everywhere * multiple local minima * a huge ridge through the middle

Gradient descent is hopeless – it gets stuck in a valley an wanders in a huge arc, never approaching even the local minima.

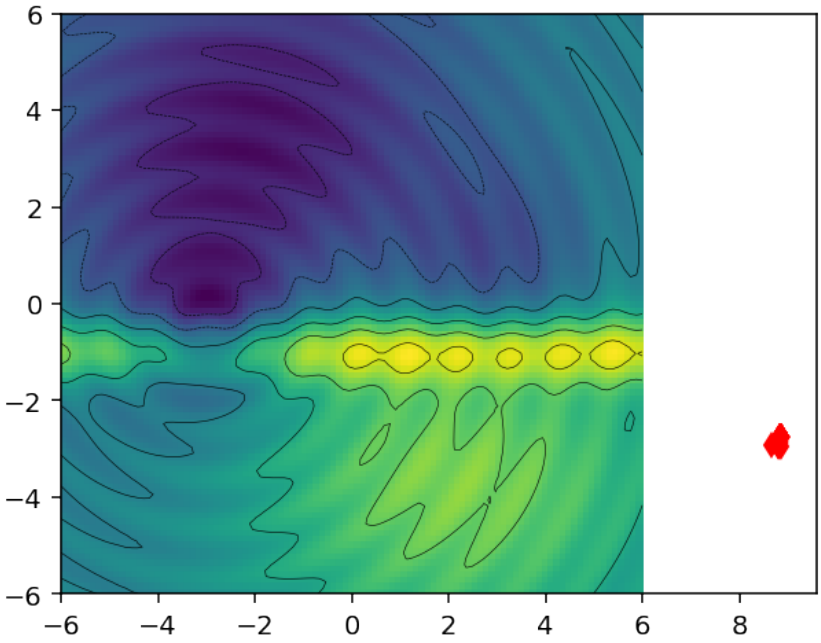
[53]:
```
# this function is crazy
# don't worry about how it is defined
# it is designed to be horrible, not realistic
def bad_function(theta):
    if len(theta.shape)==1:
        theta = theta[None,:]
    ctr = np.array([-2, 3])
    false_ctr = np.array([3,0.5])
    loss = -np.exp(-(np.sum((theta-ctr)**2, axis=1)/20.0))
    loss = loss + np.exp(-(np.sum((theta+ctr)**2, axis=1)/20.0))
    loss = loss + np.cos(np.linalg.norm(theta+false_ctr, ord=2, axis=1)*6)*0.08
    loss = loss - np.exp(-(np.sum((theta-false_ctr)**2, axis=1)/5.0))*0.75
    loss = loss - np.exp(-(np.sum((theta+false_ctr)**2, axis=1)/2.0))*0.75
    loss = loss + np.exp(-((theta[:,1]+1)**2)*2)
    return loss
```

Let's see what gradient descent does:

[58]:
```
# differentiate and do gradient descent
dbad_function = elementwise_grad(bad_function)
res = gradient_descent(bad_function, dbad_function, np.random.normal(0,4,2), 0.5)

fig = plt.figure()
ax = fig.add_subplot(1,1,1)
show_fn(ax, bad_function, (-6,6), 100, contours=50)
ax.set_aspect(1.0)

plt.plot(res.all_theta[:,0], res.all_theta[:,1], 'rd')
```

```
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:14: UserWarning: The
following kwargs were not used by contour: 'contours'
```

[58]:
```
[<matplotlib.lines.Line2D at 0x1fb3e171c88>]
```



Gradient descent cannot do a good job. Adjusting the step size can't help; the problem isn't that we've chosen a bad step size. **Stochastic gradient descent** can't help; we don't have an objective function which is a simple sum of sub-objective functions. What can we do?

7.8 Random restart

Gradient descent gets trapped in minima easily. Once it is in an **attractor basin** of a **local minima** it can't easily get out. SGD can add a little bit of noise that might push the optimiser over small ridges and peaks, but not out of deep minima. A simple heuristic is just to run gradient descent until it gets stuck, then randomly restart with different initial conditions and try again. This is repeated a number of times, hopefully with one of the optimisation paths ending up in the global minimum. This metaheuristic works for any local search method, including hill climbing, simulated annealling, etc.

7.9 Simple memory: momentum terms

A physical ball rolling on a surface is not stopped by a small irregularity in a surface. Once it starts rolling downhill, it can skip over little bumps and divots, and cross flat plains, and head steadily down narrow valleys without bouncing off the edges. This is because it has **momentum**; it will tend to keep going in the direction it was just going. This is a form of the memory metaheuristic. Rather than having ant-colony style paths everywhere, the optimiser just remembers one simple path – the way it is currently going.

The same idea can be used to reduce the chance of (stochastic) gradient descent becoming trapped by small fluctuations in the objective function and "smooth" out the descent. The idea is simple; if you are going the right way now, keep going that way even if the gradient is not always quite downhill.

We introduce a velocity v, and have the optimiser move in this direction. We gradually adjust v to align with the derivative.

$$v = \alpha v + \delta \nabla L(\theta) \theta^{(i+1)} = \theta^{(i)} - v$$

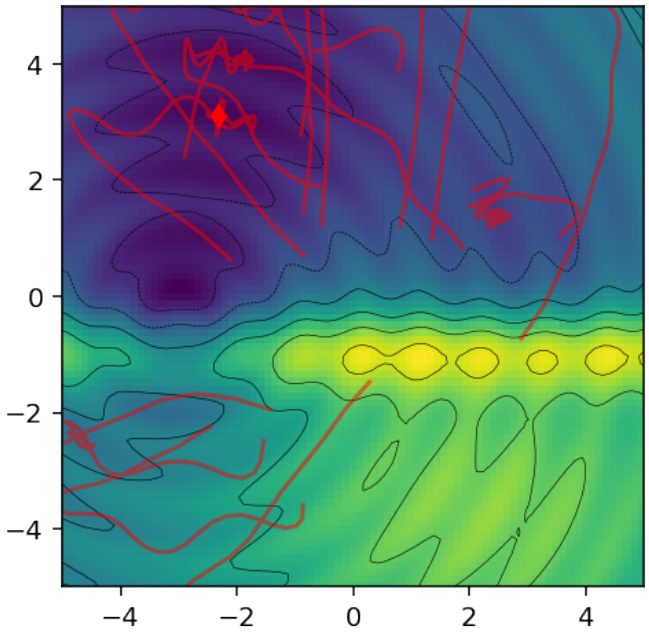
This is governed by a parameter α; the closer to α is to 1.0 the more momentum there is in the system. $\alpha = 0.0$ is equivalent to ordinary gradient descent.

[59]:
```
def gradient_descent_restart_momentum(L, dL, sample_fn, delta,
                                      alpha=0.9, restarts=20,
                                      tol=1e-4):
    o = History()
    # retry a number of times
    for i in range(restarts):
        # copy theta_0
        theta = np.array(sample_fn())
        o.loss_change = np.inf # force the optimiser to restart

        # while the loss changes
        vel = dL(theta)
        while np.abs(o.loss_change)>tol:

            # accumulate velocity "keep on rollin'"
            vel = alpha * vel +  delta * dL(theta)
            # make a step along the velocity
            theta -= vel
            o.track(np.array(theta), L(theta))

        # force a break in the plot
        o.track(np.full(theta.shape, np.nan), L(theta))
    return o.finalise()
```

[60]:
```
### now plot the trace with momentum and restarts

res = gradient_descent_restart_momentum(
    bad_function, dbad_function, lambda:np.random.normal(0,2,2),
    delta=0.2, alpha=0.9)

fig = plt.figure()
ax = fig.add_subplot(1,1,1)
show_fn(ax, bad_function, (-6,6), 100, contours=50)
ax.set_aspect(1.0)
ax.set_xlim(-5,5)
ax.set_ylim(-5,5)
ax.plot(res.all_theta[:,0], res.all_theta[:,1], 'r', alpha=0.5)
ax.plot(res.best_theta[0], res.best_theta[1], 'rd')
```

```
c:\local\anaconda3\lib\site-packages\ipykernel_launcher.py:14: UserWarning: The
following kwargs were not used by contour: 'contours'
```

[60]: `[<matplotlib.lines.Line2D at 0x1fb3d9f0550>]`



---

8 Types of critical points

This physical surface intuition leads us to think of how we would characterise different parts of an objective function.

For smooth, continuous objective functions, there are various points in space of particular interest. These are **critical points**, where the gradient vector components is the zero vector. *Image: classification of critical points. Each of these corresponds to a different configuration of the eigenvalues of the **Hessian**.*

8.1 Second-order derivatives

If the first order derivatives represent the "slope" of a function, the second order derivatives represent the "curvature" of a function.

For every parameter component θ_i the Hessian stores how the *steepness* of every other θ_j changes.

Imagine I am on a hill. * The altitude I am at is the value of the objective function. * The parameters I can vary are my position North/South and East/West. * The gradient vector is the change in altitude as I take a step North or a step East, which are the two parameters. This is the local

steepness at the place I am at on the hill. * The Hessian captures how much steeper the hill get stepping Northwards as I go North and *also* how much steeper the hill gets Eastwards as I step North; similarly for stepping East. So there is a 2x2 matrix describing these changes in steepness.

For a vector valued function $f(\vec{x})$, then we have:

$$\nabla L(\vec{\theta}) = \left[\frac{\partial L(\vec{\theta})}{\partial \theta_1}, \frac{\partial L(\vec{\theta})}{\partial \theta_2}, \ldots, \frac{\partial L(\vec{\theta})}{\partial \theta_n}\right],$$

the gradient vector, and the second order derivatives are captured by

$$\nabla\nabla L(\vec{\theta}) = \nabla^2 L(\vec{\theta}) = \begin{bmatrix} \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1^2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1 \partial \theta_2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1 \partial \theta_3} & \cdots & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_1 \partial \theta_n} \\ \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2^2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2 \partial \theta_3} & \cdots & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_2 \partial \theta_n} \\ \cdots & & & & \\ \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n \partial \theta_1} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n \partial \theta_2} & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n \partial \theta_3} & \cdots & \frac{\partial^2 L(\vec{\theta})}{\partial \theta_n^2} \end{bmatrix},$$

the **Hessian matrix**. Note that we have an entry in the Hessian matrix for every *pair of dimensions* in the function. You might notice the similarity to the covariance matrix, which captured how data coordinates varied with each other; the Hessian matrix captures how gradients of a function vary with each other.

For a 2D surface, the gradient vector specifies the normal of the plane tangent to the surface at a given point. The Hessian matrix specifies a quadratic function (a smooth curve with one minima) following the curvature of the surface.

8.1.1 Eigenvalues of the Hessian

The Hessian matrix captures important properties about the **type of critical point** that we saw in the previous lecture. In particular, the **eigenvalues** of the Hessian tell us what kind of point we have.

- If all eigenvalues are all strictly positive, the matrix is called **positive definite** and the point is a minimum.
- If all eigenvalues are all strictly negative (**negative definite**) and the point is a maximum.
- If eigenvalues have mixed sign the point is a saddle point.
- If the eigenvalues are all positive/negative, but with some zeros, the matrix is **semidefinite** and the point is plateau/ridge.

8.2 Second-order optimsation

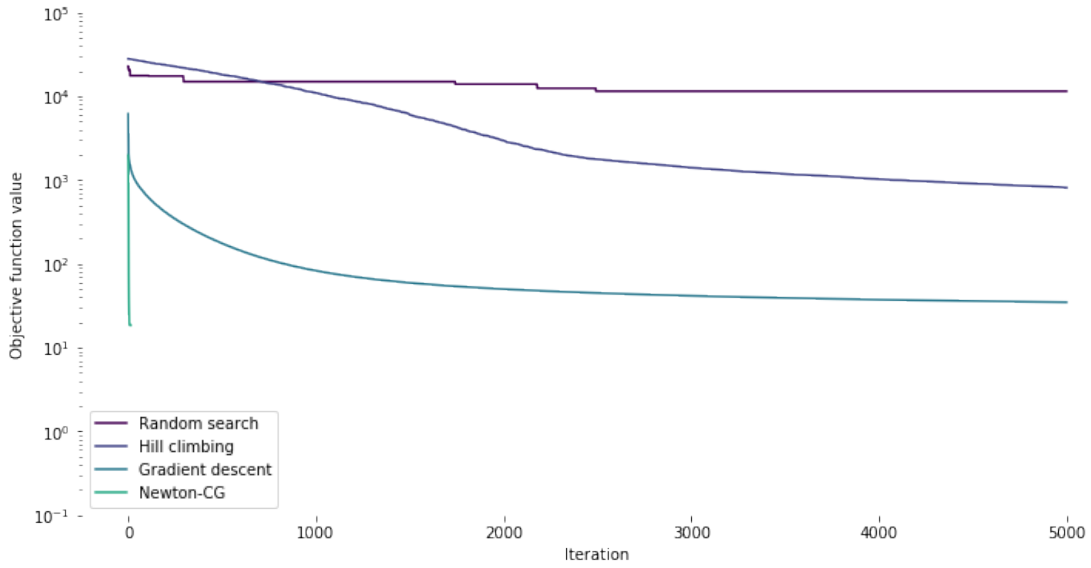
Second-order optimisation uses the Hessian matrix to jump to the bottom of each local quadratic approximation in a single step. This can skip over flat plains and escape from saddle points that slow down gradient descent. Second-order methods are *much* faster in general than first-order methods.

[61]:
```
from autograd import grad, jacobian
from utils.optimisers import random_search, hill_climbing,  gradient_descent
import scipy.optimize
import autograd.numpy as np
```

```
# the linear regression problem; find m and c in the equation y=mx+c
dim = 15
x = np.sort(np.random.normal(0,1,(20,dim)))
A = np.random.normal(0,1,(dim,dim))
b = np.random.normal(0,10,(dim,))

y = (x@A) + b + np.random.normal(0, 0.5*np.abs(x), x.shape)
l = len(A.ravel())
params = l + len(b)
%matplotlib inline
%matplotlib inline

import matplotlib.pyplot as plt

def loss(theta):
    # sum of squares
    Ap = theta[:l].reshape(A.shape)
    bp = theta[l:]

    e = np.sum(((x @ Ap + bp) - y)**2)
    return e

# compute derivative (in one step!)
dloss = grad(loss)

guess = lambda: np.random.normal(0, 1, params)
neighbour = lambda x: x+np.random.normal(0, 0.01, params)

random_res = random_search(loss, guess, 5000)
hill_res = hill_climbing(loss, guess, neighbour, 5000)

gd_res = gradient_descent(loss, dloss, guess(), 1e-3, maxiter=5000)

ncg_trace = []
def record_trace(x):
    ncg_trace.append(loss(x))
ncg_res = scipy.optimize.minimize(fun=loss,
                                  x0=guess(),
                                  callback=record_trace,
                                  method='Newton-CG',
                                  jac=grad(loss),
                                  hess=jacobian(grad(loss)))


fig = plt.figure(figsize=(12,6))
ax = fig.add_subplot(1,1,1)
```

```
ax.plot(random_res.loss_trace, label="Random search")
ax.plot(hill_res.loss_trace, label="Hill climbing")
ax.plot(gd_res.loss_trace, label="Gradient descent")
ax.plot(ncg_trace, label="Newton-CG")

ax.set_frame_on(False)
ax.set_yscale("log")
ax.set_ylim(1e-1, 1e5)
ax.legend()
ax.set_xlabel("Iteration")
ax.set_ylabel("Objective function value")
```

[61]:
```
Text(0, 0.5, 'Objective function value')
```



Curse of dimensionality (yet again) However, simple second order methods don't work in high dimensions. Evaluating the Hessian matrix requires d^2 computations, and d^2 storage. Many machine learning applications have models with $d > 1$ million parameters. Just storing the Hessian matrix for *one iteration* of the optimisation would require:

Second order optimisation can move much more quickly through saddle points and plateaus than first order methods like gradient descent. It can be particularly effective in low-dimensional problems, but the **curse of dimensionality** always has its way. Imagine we have a 1 million parameter problem to optimise. The gradient vector would have as many elements as the parameter vector; so 1 million elements, or about 8 megabytes of memory requirement for `float64`. But the Hessian matrix has to store the change in every *pair* of parameters. This would take:

[ ]:
```
print("{0} bytes of memory".format(1000000 * 1000000 * 8)) # 8 bytes per float
```

which is 8 terabytes! This is an impossible computational burden. There are special, limited-memory forms of second order methods, which use approximate Hessians (like the widely used L-BFGS algorithm) but these are outside the scope of this course.

8.3 Resources

- **How machines learn** **Recommended: WATCH THIS**
- **What is backpropagation** if you want more detail on how first-order optimisation is used in deep learning.
- **Gradient based optimization**
- **An overview of gradient descent optimization algorithms**
- **An introduction to algorithms for continuous optimization** by Nicholas Gould
- **Khan academy: Multivariable calculus**, particularly "Thinking about multivariable functions", "Derivatives of multivariable functions" and "Applications of multivariable derivatives"

8.3.1 Beyond this course

- **When least is best: How Mathematicians Discovered Many Clever Ways to Make Things as Small (or as Large) as Possible** *by Paul J. Nahin* An interesting and mathematically thorough description of the history of optimisation from a mathematical standpoint.