Unconstrained Numerical Optimization
An Introduction for Econometricians

Lecture Note
Advanced Microeconometrics
Anders Munk-Nielsen
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Abstract

This note introduces unconstrained numerical optimization. The intention is to allow the user to understand the output from Matlab when using `fminunc` and `fminsearch` as well as the options available in the powerful set of tools behind. After a short introduction, gradient-based optimization algorithms are covered, followed by gradient-free algorithms. After this, an example in Matlab is introduced, where the Rosenbrock function is minimized using both types of optimizers. The gradient-based optimizer is superior to the gradient-free, but we also consider a "noisy" Rosenbrock function where the gradient-free optimizer outperforms the gradient-based one. The note is concluded with some practical advice in Section on troubleshooting when optimization fails, debugging code and making the code run faster.

The note is structured with the intention that details can be skipped if the reader is not interested in them. The example in Section 4 will illustrate how the optimization theory works in practice in Matlab and in particular give an example where it does not work and explain why. Section 5 is intended to be used for quick and easy reference when things go awry.

Contents

1 Introduction

In this note, we will consider the problem,

$$\min_x f(x). \tag{1}$$

Note that any maximization problem can be turned into a minimization problem by minimizing -1 times that function, so it is completely general. The formulation nests M-estimators directly, for example the likelihood function can be written as the minimization problem,

$$\min_\theta N^{-1} \sum_{i=1}^{N} -\log l(\theta|y_i, x_i),$$

where (y_i, x_i) is data for observation i and l is the likelihood function. To make notation simpler to read, we will subsume the average in this note and just work with a function f. Note that in most econometric applications, the objective will also be a function of data (like y_i and x_i above), but this is kept fixed throughout estimation, so we only consider the objective as a function of parameters.

Throughout this note, we will be discussing methods for finding *local optima*. In general, there is no way of ensuring that one has found the global optimum (in fact, it can be proven that unless one's algorithm visits every single x with some positive probability, this can never be guaranteed). The only generally accepted method for ensuring that the *global* optimum has been found is using a *multi-start procedure*, where the optimization algorithm is started at many different initial values.

Optimizers fall into two overarching groups;

1. Gradient-based (`fminunc` in Matlab),
2. Gradient-free (`fminsearch` in Matlab).

The Nelder-Mead algorithm (which is implemented in `fminsearch`) is the only example of a gradient-free optimizer that will be discussed herein. From personal experience, gradient-based optimizers are faster but require the problem to be "nicer" (i.e. more smooth, look more like a polynomial). The Nelder-Mead algorithm is typically very useful when the starting values are bad or the problem is difficult, e.g. if complicated calculations are involved which might result in roundoff error, producing noise in the evaluation of f.

We start by discussing gradient-based methods and then turn to a brief discussion of the Nelder-Mead algorithm in the end. Table 1 gives an overview of the optimizers we will cover.

Table 1: Overview of optimizers

	Newton	BFGS	BHHH	Nelder-Mead	Steepest Descent
Matlab	User written	`fminunc`	`fminunc`	`fminsearch`	`fminunc`
Option	–	[default]	Provide user-written Hessian		`HessUpdate ='steepdesc'`
Gradient used	✓	✓	✓	÷	✓
Hessian used	✓	✓	✓	÷	÷
Step	$f'(\cdot)/f''(\cdot)$	$f'(\cdot)/f''(\cdot)$	$f'(\cdot)/f''(\cdot)$	Heuristic	$\gamma f'(\cdot)$
Hessian	Numeric	Iterative updating	Outer product	Not used	Not used
Best for	Nice f but weird Hessian	Nice f	Likelihood estimation	Nasty f	Non-convex or non-quadratic f
Computationally	Medium cost	Cheap	Cheap	Expensive	Expensive
Globalization	Line search	Line search	Line search	n.a.	Line search

2 Gradient-based Optimization

Intuitively, one can think of the core step of an optimization problem as: given an initial point x_0, what is our best guess of the minimizing value of x? In other words, what should the next value of x be. Most methods rely both on the *slope* and *curvature* of the function at x_0 (i.e. first and second derivatives). The exception is the steepest descent method, which only relies on the first derivative.

2.1 Steepest Descent Methods

The steepest descent (also called gradient descent) algorithm relies only on the first-derivatives of f at x_o. It looks at the slope of f and moves downhill. The challenge is how far to go. If we just keep taking tiny steps downhill, we will eventually reach a local minimum. However, it may take very long for us to get there. Therefore, the step we take is simply proportional to the derivative, i.e. for $x \in \mathbb{R}^1$,

$$x_1 = -\gamma f'(x_0),$$

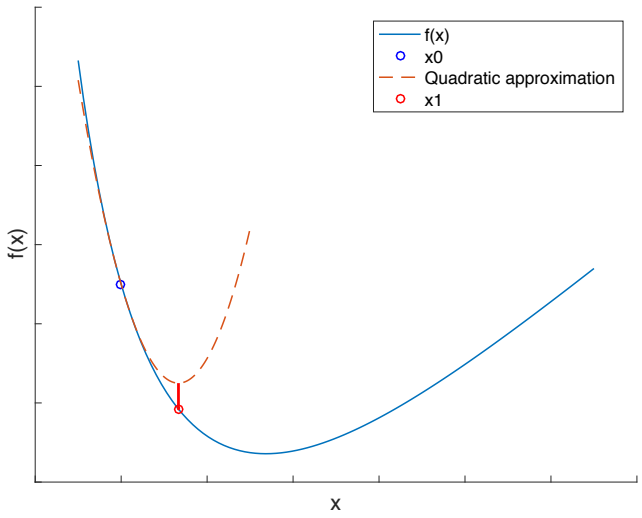
and for vector-valued x,

$$x_1 = -\gamma \nabla f(x_0).$$

The *step size*, γ, is allowed to change with every iteration. It is typically chosen based on *line searching*, outlined in Section 2.5.

The algorithm can be awfully slow. In the example in Section 4.2, the steepest descent algorithm requires 56,649 function evaluations to do find the minimum, compared to just 20 function evaluations for the default newton-based algorithm. The gradient descent algorithm is simple to understand but is almost always outperformed by Newton-based algorithms. Except in the case of highly non-quadratic or non-convex problems; in those cases, the Hessian is not at all informative about where to go whereas the gradient descent algorithm will just

Figure 1: Function with Quadratic Approximation



keep going down hill.

2.2 Newton-based Methods

To do this, we will form a 2nd order Taylor approximation to f and set the next x to be the minimizer for that approximation. A 2nd-order Taylor approximation is the best quadratic function that approximates f in a neighborhood of x_0. Once we have taken the step and gone to the x that minimizes the quadratic approximating function, we will form a new approximation at this new value of x and proceed in that manner until we arrive at a stationary point (i.e. where the gradient is the zero vector). In Table 1, it says that the Newton-based optimizers (Newton, BFGS, BHHH) work well when "f is nice". What is meant by this is that the function cannot be too far from a quadratic function and should in particular be convex (most places). If f is very far from a quadratic function, of course the quadratic approximation will be poor and we are in trouble.

Let us start by considering the simplest version of the problem where x is a scalar. Then the approximating quadratic function that we are minimizing is

$$\min_{x\in\mathbb{R}} f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2.$$

Figure 1 illustrates this graphically. We are constructing a quadratic function that at the point x_0 has the same slope as f, namely $f'(x_0)$, and the same curvature, $f''(x_0)$, and then we move to the bottom of this function and assign our new iterate, x_1, to the x-value here.

In the more general, x is a $P \times 1$ vector, and the problem takes the form

$$\min_{x \in \mathbb{R}^P} f(x_0) + \nabla f(x_0)'(x - x_0) + \frac{1}{2}(x - x_0)'\nabla^2 f(x_0)(x - x_0).$$

Here, $\nabla f(x_0)$ is the $P \times 1$ vector of first derivatives (called the *gradient*), so that the term $\nabla f(x_0)'(x - x_0)$ is scalar. The Hessian matrix, $\nabla^2 f(x_0)$, is the $P \times P$ matrix of 2nd derivatives, so the last term is a quadratic form and therefore also scalar. Alternatively, we may formulate the model in terms of the *step*, which we can write as $s \equiv x - x_0$, and the problem becomes

$$\min_{s \in \mathbb{R}^P} f(x_0) + \nabla f(x_0)'s + \frac{1}{2}s'\nabla^2 f(x_0)s. \tag{2}$$

Intuitively, when we replace (1) with (2), we are finding the quadratic function (2nd-order polynomial) that is the best approximation to f at the point x_0. Then we minimize that function rather than the original f. Therefore, if f is locally concave, we will go in the wrong direction. Similarly, if f is highly "non-quadratic" (so that the third term in the Taylor expansion is very important), the approximation is very poor and we may for example "over-shoot" and take a too long step. To avoid these problems, the quadratic optimization problem (2) should be accompanied by a *globalization strategy*; this is a way of trying to avoid overshooting (and sometimes also undershooting; then it is called a *greedy* globalization strategy). See Figure 2 for an example where the function is locally very non-quadratic at x_0, resulting in the quadratic approximation overshooting the minimum. Intuitively, the gradient and Hessian of f will give us a *direction* along which we will search for candidate improvements. We will first try the most obvious candidate, but if that turns out not to result in an improvement, the globalization strategy will indicate how we should proceed.

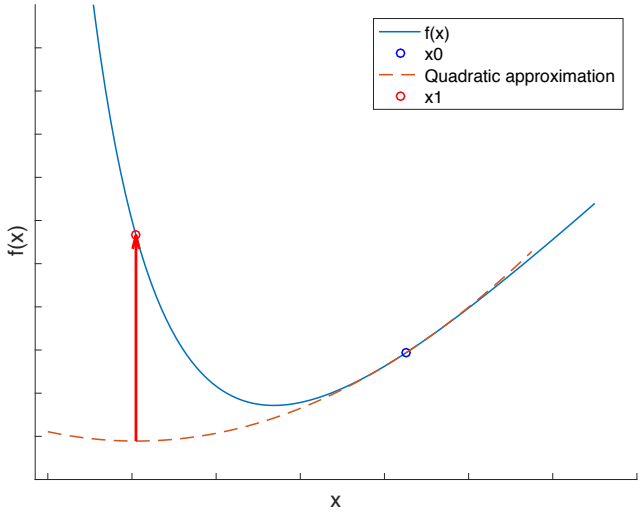
You may be wondering why we only choose a quadratic approximation to the true function and do not proceed to a cubic (3rd-order Taylor approximation) or even higher. The reason is that minimizing a quadratic function is very simple and requires only linear algebra, which is extremely fast. Going to a higher-order polynomial would require us to do a more complex optimization problem to minimize the approximating function, which defeats the purpose of minimizing a local approximating function.

In order to come up with an algorithm, we will now need to do decide on three components;

1. How to choose the step, s,
2. A globalization strategy,
3. A method for minimizing the quadratic function.

Let us postpone the globalization strategy for a while and focus on the other two. We will first discuss the scalar case, then consider the vector case and finally we will add the globalization strategy.

Figure 2: Local Non-quadraticness Leading to Overshooting



2.3 Scalar x, no globalization strategy

In the simplest case, we are solving the problem

$$\min_{s\in\mathbb{R}} f(x_0) + f'(x_0)s + \frac{1}{2}f''(x_0)s^2.$$

Interior solutions will satisfy the first-order conditions,

$$\begin{aligned} \Rightarrow \text{FOC} : f'(x_0) &= -f''(x_0)s \\ \Leftrightarrow s &= -\frac{f'(x_0)}{f''(x_0)}, \end{aligned} \tag{3}$$

assuming that $f''(x_0) \neq 0$. The intuition is that $f'(x_0)$ gives the direction while $f''(x_0)$ tells us how large of a step, we should take; when $f'(x_0) < 0$, the function slopes downwards and we should take a step in the positive direction in order to reduce the function value (and vice versa). When $f''(x_0)$ is small (but positive), it means that the slope of f only changes very slowly, indicating that we should be taking a larger step (and vice versa).

2.4 Vector x, no globalization strategy

Consider the case where $x \in \mathbb{R}^P$. Here, the first-order conditions necessary for interior solutions to (2) yield

$$\text{FOC} : \nabla f(x_0) = -\nabla^2 f(x_0)s.$$

If f is strictly convex at x_0, then $\nabla^2 f(x_0)$ is positive definite and we can invert the equation no obtain

$$s = -[\nabla^2 f(x_0)]^{-1} \nabla f(x_0). \tag{4}$$

This is simply the vector-generalization of (3) and the intuition is the same.

Even though the inversion in (4) is feasible theoretically, it may become computationally costly if P is large to invert the $P \times P$ system. There exists different methods for doing this;

- Cholesky method,
- Conjugate gradient method.

Both methods are computationally superior to finding the inverse of the Hessian as in (4) and yield almost identical solutions. The Cholesky method is a more direct method whereas the conjugate gradient method iteratively computes candidate solutions that become better successively. When P is large, the Cholesky method may be slow and the conjugate gradient method will speed things up. This is applicable if the evaluation of f is generally very fast (several evaluations per second). For most econometric problems, it is not important.

If f is non-convex, then we may not be able to invert the equation. Similarly, if our numerical calculation of the Hessian is poor, we may get trouble with finding the step size in equation (4). In these cases, it is generally advisable to check for errors in the code that calculates f and otherwise maybe try to see if a gradient-free optimizer can break free of the locally non-convex area. There are alternative methods for dealing with the inversion in the case of non-positive definite Hessian matrices, but the general advice is to hope that the problem disappears as we get towards the minimum.

A computational note: One should **never** actually calculate the inverse of the Hessian. This is a waste of computational resources. Instead, the system above can solved in Matlab by writing

$$\texttt{s} = -\texttt{hessian}\backslash\texttt{gradient}.$$

The "backslash" operator solve linear systems of the form $As = b$ for s, where A is $P \times P$ and s, b are $P \times 1$. It never actually computes the inverse, A^{-1}; when A is positive definite, one can find a lower triangular L such that $A = LL'$ and find $s = (L')^{-1}L^{-1}b$, which is computationally far simpler.

2.5 The Line Search Algorithm

The intuition in the line search algorithm is that we search for the optimal step along the one-dimensional line indicated by (4). That is, we choose the step

$$s = -\lambda[\nabla^2 f(x_0)]^{-1} \nabla f(x_0),$$

where $\lambda > 0$. Typically, we start out with $\lambda = 1$ and if that fails, we try $\lambda = 0.5$, then $\lambda = 0.25$, etc. If the problem is highly non-convex and has a very small Hessian locally, then it may result in s being too large and dampening it with $\lambda < 1$ can then help. This approach is known as the "backtracking Armijo line search". If one implements a "greedy" version of the line search, it could also be possible to experiment with $\lambda > 1$ but that is not the standard case; the primary purpose of the line search is to avoid situations where we overshoot the minimum and end uphill anyway. Figure 2 illustrates such a case of overshooting; note how the objective function does not change much at the initial point (low Hessian). This is the non-quadraticness that results in the too large step.

If it is not possible to find an improvement this way (the algorithm typically terminates when $\lambda < 10^{-6}$ in Matlab), then the optimizer gives up. In Matlab, this results in the error message:

> `fminunc stopped because it cannot decrease the objective function along the current search direction.`

In that case, try starting `fminsearch` to see if it is, e.g., a local non-convexity problem, which the gradient-free optimizer can break free of.

There are alternative implementations of the line search where one requires not only a decrease in f, but a *sufficiently large* decrease in f according to some inequality. This results in a rule for whether or not to *accept* any proposed step by the algorithm.

2.6 The Trust-region Method

The idea is similar to the line search algorithm in that we want to avoid the optimizer taking a huge step and overshooting the true minimum. Instead of searching for the optimal step size, the trust-region restricts the range of s-values that we search for in the quadratic problem, replacing (2) with the *constrained* quadratic problem

$$\begin{aligned} &\min_s f(x_0) + \nabla f(x_0)'s + \frac{1}{2}s'\nabla^2 f(x_0)s, \\ &\text{s.t.} \quad \|s\| \leq \Delta, \end{aligned} \tag{5}$$

where Δ is the trust region's *radius*. Note that the constraint defines a ball in $\mathbb{R}^P$ if the Euclidean norm (the typical distance), $\|\cdot\|_2$ is used. A trust-region algorithm now requires two more ingredients,

1. A method for solving the constrained quadratic program (5),
2. A rule for updating Δ.

There are many linear algebra methods for solving such problems and since they will not be the computational bottleneck in typical econometric applications, we will not worry about

them here. The rule for updating the radius will be based on a comparison of the realized decrease achieved in f after taking the step compared to the "expected decrease in f" (this latter bit of course requires some model). If the decrease is smaller than expected, the radius is increased and vice versa.

2.7 Gradients

No matter the choice of globalization strategy, both the line search and the trust region relies on a gradient vector, $\nabla f(x_0)$, and a Hessian matrix, $\nabla^2 f(x_0)$. In this section, we cover the gradient and in the next section the Hessian.

There are generally two methods for obtaining the gradient;

1. Analytic gradient (more precise, but costly in human computational time),
2. Numerical gradient (using some finite-difference approximation).

Generally, the analytic gradients are preferable if they are available but it can take time to code them up and verify their correctness. Using analytic gradients tends to result in more precise and faster optimization. Additionally, optimization will be more robust to numerical error in the evaluation of f (so long as the same error is not present in the evaluation of ∇f). Below is an example where the Rosenbrock function has been coded in Matlab and includes the gradient (which has two elements because the input, `x`, should have two elements).

```
function [f,g] = rosenbrock(x)
% Returns the Rosenbrock function with gradients.
% Note: x should have two elements.
f = 100*(x(2) - x(1)^2)^2 + (1-x(1))^2;
if nargout > 1 % Computed if the gradient is required
    g(1) = -400*(x(2)-x(1)^2)*x(1)-2*(1-x(1));
    g(2) =  200*(x(2)-x(1)^2);
end
```

When gradients are not supplied analytically in Matlab, the optimizer will obtain them using numerical differentiation. That is, it will approximate it by

$$\left.\frac{\partial f}{\partial x_k}\right|_{x=x_0} \cong \frac{f(x_1)-f(x_0)}{h}, \quad \text{where } x_{1j} = \begin{cases} (1+h)x_{0j} & \text{if } j=k \\ x_{0j} & \text{otherwise.} \end{cases} \tag{6}$$

That is, x_1 is the same as x_0 except at the coordinate to the entry, which we are taking the derivative with respect to. Note that the step is *relative* — this is by far superior to using the same absolute step regardless of the magnitude of each x_{0k}. The finite difference in (6) is a *forward difference*; alternatively, one can use a *centered difference*, which is more precise

but requires two evaluations of the objective function for each parameter (so $2P$ evaluations), which is often too expensive to be preferable. Instead, (6) re-uses $f(x_0)$ (which can also be supplied to the gradient calculator) and thus only requires $P + 1$ evaluations.

Generally speaking, the step size should be set to

$$h^* = \sqrt{\epsilon},$$

where ϵ is *machine precision*. This can be obtained in Matlab with the built-in variable `eps`, which shows that

$$\epsilon = 2.2204 \cdot 10^{-16}.$$

This is the distance in floating point arithmetic (how the computer represents numbers) between 1 and the closest number on the real line in the positive direction. That is, if you type `1 + eps/2`, you will get precisely 1 (in fact, `1 + eps/x` for any `x>1` will return just `1`). Since there are 52 bits available to represent the number, $\epsilon = 2^{-52}$.

Why is it then optimal to choose $h = h^*$? This is because with finite differences, there are two sources of error:

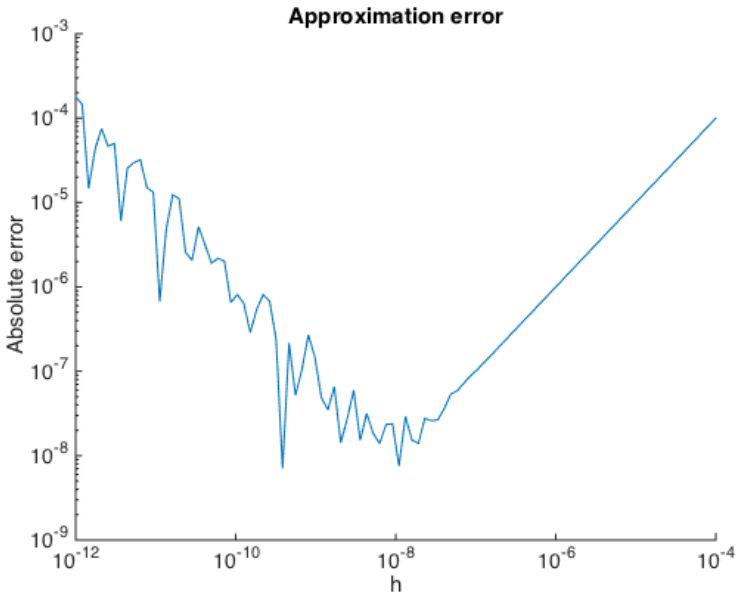
1. Approximation error,
2. Roundoff error.

The first error comes from the fact that we are using a finite difference approximation. As you may recall from basic calculus, the true derivative at the point x_0 is the *limit* of the forward differences in (6) when $h \to 0$. The second source of error is perhaps new to many economists and comes from the fact that a computer cannot represent all the real numbers and therefore makes roundoff error. This problem becomes particularly bad when the numbers we operate on are extremely small (such as subtractions between numbers that are very close or division by very dis-similar numbers). In the subsection below, we will discuss this more and consider what h will optimally balance these two errors off. The general rule of thumb is to choose $h = 10^{-8}$, which is also (close to) the default in Matlab. If the function is very complicated and involves many steps that might lead to roundoff error, it may be advisable to work with a larger step size, e.g. $h = 10^{-6}$, because the approximation error may be much larger in that case.

2.7.1 Optimal Step Size h

Let us first try to understand roundoff error better. It comes from the fact that the computer works with finite precision. Not every single real number can be represented in the computer's memory. Instead, it will constantly be choosing the closest number to the ones it can to the ones we ask it to store (*some* numbers of course coincide and luckily, for example all the

Figure 3: Approximation Error and the Choice of h



natural numbers are among such). For example, in Matlab

$$\texttt{10} + \texttt{eps} - \texttt{10} = \texttt{0},$$

because the number $\texttt{10} + \texttt{eps}$ cannot be represented in machine precision. However,

$$\texttt{10} - \texttt{10} + \texttt{eps} = \texttt{2.2204e-16},$$

so the sequence of operations matters when working with numbers on a computer. It turns out that in particular subtraction and division can cause problems on a computer. So *the smaller the number we are dividing by and the closer the numbers we are subtracting, the larger the roundoff error*. This is why we should not set h too small. Figure 3 shows the approximation error in a finite difference approximation to the derivative of the function $f(x) = x^2$ at $x_0 = 1$ for different choices of h. On the right hand side, the error is dominated by the *approximation error* (and it appears to be a smooth function in h). On the left hand side, it is dominated by *roundoff error* (and that error looks much more jittery and unexpectable, as one might suspect).

2.8 Hessian

There are three ways in which to obtain the Hessian:

1. Analytic Hessian,

2. Clever updating schemes (e.g. the BFGS),

3. Using an approximation (e.g. the BHHH),

4. Numerical Hessian.

The analytic Hessian is obtained by doing derivatives with pen and paper (or with some symbolic mathematics software, like Maple), and coding them up as a part of the criterion function. From personal experience, it is not simply the case that the the analytic option is always better. Mainly because it is extremely time-consuming to derive the Hessian analytically and very hard to verify that it has been done correctly.

In the other extreme, the fully numerical Hessian is easy to use because it is always available; we just take finite differences of the finite differences (essentially using equation (3) P times for each of the P entries in the gradient). However, it is costly to evaluate using finite differences, requiring P^2 evaluations of the f function. This is why in Table 1, it says that the pure Newton method is medium-costly; it might get to the minimum in a low number of *iterations*, but at each step, it will have to evaluate the objective function P^2 times in order to obtain the Hessian.

In between these two extremes are the BFGS updating scheme and the BHHH approximation. The BHHH algorithm uses an approximation to the Hessian that relies on the gradient only. The approximation is only valid in certain models, most notably maximum likelihood. The BFGS algorithm is the default version in `fminunc` (Matlab's standard optimizer). It uses information on the current and previous x and ∇f to make an informed guess as to what the Hessian is. The BFGS algorithm turns out to perform extremely well in practice for a surprisingly wide class of optimization problems. In the following two subsections, we will discuss the BFGS updating scheme and the BHHH Hessian approximation. The finer mathematical details of the BFGS algorithm are not required exam knowledge; only an intuitive understanding is required.

2.8.1 BFGS

The standard implementation of the unconstrained optimizer, `fminunc`, in Matlab uses the BFGS updating scheme (named after Broyden, Fletcher, Goldfrab and Shanno). This, and other updating schemes like it, consists of using the gradient from the current and the previous iterations to construct an informed guess as to what the Hessian might look like. Specifically, the BFGS approximates $\nabla f(x_0)$ by the matrix H_0. This matrix can be initialized to be the identity matrix. Then when the step, s, has been found (subject to the globalization rule, line search or trust region), the updated Hessian, H_1, is constructed as

$$H_1 = H_0 + \frac{1}{y's} yy' - \frac{1}{s'H_0 s} H_0 ss' H_0,$$

where $y \equiv \nabla f(x_0 + s) - \nabla f(x_0)$.[1] The main advantage of the BFGS approximation of the Hessian is that it requires no additional evaluations of f in excess of what is already being done, it merely requires us to store the previous gradient's value. The update step for the Hessian just requires linear algebra, which will typically be so fast that the total computational time is unaffected since in general in econometric applications, the dimension of P is so low that it is almost only the evaluation of f that is computationally costly.

In Table 1 it says that the BFGS works well when the function f is nice, whereas the pure Newton algorithm also works well when the Hessian is weird. What I mean here is that it might for example be the case that the Hessian of the objective function changes a lot when x changes; in that case the updating scheme used by BFGS might not work that well and it might be better to actually calculate the numerical hessian at each new point, x.

2.8.2 BHHH

The BHHH is an important algorithm for estimating likelihood models. It was first proposed by Berndt, Hall, Hall and Hausman (1974), and it uses the average outer product of the scores as an approximation to the expected Hessian. This approximation is only applicable when f takes the form of a sum (or equivalently, an average), i.e.

$$f(x) = N^{-1} \sum_{i=1}^{N} q(w_i, x),$$

(recall that x plays the role of parameters, which we otherwise label θ, and w_i is individual i's data) and when either q is the likelihood function so that the *information matrix equality* is satisfied (which it always is for maximum likelihood) or q and the model structure is such that the *generalized information matrix equality* is satisfied. In that case, the Hessian can be approximated by

$$\nabla_x^2 f(x) \cong N^{-1} \sum_{i=1}^{N} \nabla_x q(w_i, x)' \nabla_x q(w_i, x),$$

where the inner term is the outer product of the scores.[2] Thus, the BHHH step becomes,

$$s = - \left[N^{-1} \textstyle\sum_{i=1}^{N} \nabla_x q(w_i, x)' \nabla_x q(w_i, x) \right]^{-1} \left[N^{-1} \textstyle\sum_{i=1}^{N} q(w_i, x) \right].$$

[1] As a side-note, both the matrices yy' and $H_0 ss' H_0$ have rank 1 and are symmetric. Together, they form a rank 2 update of the Hessian.

[2] Essentially, the information matrix equality states that the expected value of the Hessian matrix (times a scalar) is equal to the expected value of the outer product of the scores, i.e.

$$\sigma_o^2 \mathbb{E} \left[\nabla_\theta^2 q(w, \theta_o) \right] = \mathbb{E} \left[\nabla_\theta q(w, \theta_o)' \nabla_\theta q(w, \theta_o) \right],$$

where θ_o denotes the true minimizing parameters (x throughout the rest of this note). The equation is discussed in Wooldridge (2010; p. 417).

The approximation has the clear advantage that since we aldready calculated gradients, no additional evaluations of the criterion function are required. However, it does require us to store the criterion value *for each observation*, which we might not otherwise be doing. In other words, we cannot use the gradient that comes out of `fminunc` to construct this outer product of the scores.

In the context of maximum likelihood, this approximation works when *i)* we are close to the true parameters, *ii)* the sample size, N, is large, and *iii)* the model is correctly specified. For example, if the starting values are very bad, this may result in poor performance.

2.9 Termination

The optimization algorithm can terminate for a number of reasons;

1. Gradients are sufficiently close to zero,
2. Change in x is too small,
3. Change in f is too small,
4. Step size too small (line search or trust region radius failure),
5. Maximum iterations reached.

Only termination due to criterion 1 is truly satisfactory, since the necessary condition for interior optimum is gradients being equal to zero. From that point of view, it seems strange that it should be possible to converge to a point where gradients indicate a slope of the function, but where the optimizer fails to decrease the function value along the direction (termination due to 2, 3 or 4). One possible explanation in this case is that there is a problem with the gradients. If there is numerical noise (roundoff error) in the function, then perhaps increasing the step size for the numerical gradients might yield a better gradient approximation. It might also be that the optimizer has gotten stuck in a local minimum or a local non-convexity. In that case, try using a gradient-free optimizer for a few iterations to see if it can break out of such a local problematic area.

The default maximum iterations in Matlab is 300. If the optimizer terminates due to criterion 5, the obvious solution is to just provide more iterations. Generally, econometric problems can be much less well-behaved than the simple analytic functions studied in the optimization literature. In particular when the starting values are bad.

3 Gradient-free Optimization

The Nelder-Mead method or the Simplex method is an optimization algorithm that does not rely on gradients. Its theoretical properties are much poorer than those of gradient-based

optimizers; for example, once a gradient-based optimizer gets within the "region of attraction" of the true minimizer, quadratic convergence kicks in. This means that the distance to the truth will be doubling the exponent, e.g. $10^{-1}, 10^{-2}, 10^{-4}, 10^{-8}$. No similar theoretical results hold for the simplex algorithm, so it tends to use a lot of steps to get the final distance covered. This is why it says in Table 1 that the algorithm is computationally costly. Each individual iteration it takes requires only a single evaluation of the objective function, but it typically takes many many more iterations than the Newton-based solvers.

The simplex algorithm works by always keeping track of $P+1$ points, $\{(x_p, f(x_p))\}_{p=1}^{P+1}$; such a structure is called a simplex, hence the name. Intuitively, the algorithm then keeps moving away from the point that is the highest (i.e. the worst point). If the algorithm sense that it's moving in a good direction, it will be "expanding" the simplex, taking bigger and bigger steps. When it encounters non-improvements in the direction of the lowest point, it will instead be shrinking the simplex points towards the lowest one. If you google Nelder-Mead, there are plenty of youtube videos and GIF illustrations to show examples of the optimizer at work to aid the intuition of how it functions.

The termination criteria will naturally not involve gradients; the algorithm only terminates if

1. The change in f is sufficiently small (default 10^{-4}),
2. The change in x is sufficiently small (default 10^{-4}),
3. Maximum iterations have been reached (default is $200P$).

Naturally, the third is not a satisfactory termination message. However, since the simplex algorithm can be used very effectively to break free of local minima or areas of non-convexity, you may find it useful to be starting `fminsearch` with a small number of iterations and then proceeding with a gradient-based optimizer in `fminunc` afterwards. In the following section, the specific details of the algorithm is presented.

3.1 More Details

This section lays out the precise details of the Nelder-Mead algorithm. These details are not required exam knowledge but to satisfy the curious reader.

Algorithm (Nelder-Mead).

1. Order the points in order of function value,

$$f(x_{(1)}) \leq \cdots \leq f(x_{(P+1)}).$$

2. Compute the *centroid*, $\overline{x}$, as the average of all points except the worst,

$$\overline{x} = P^{-1} \sum_{p=1}^{P} x_{(p)}.$$

3 (reflexion). Compute the *reflected point*,

$$x^r = \overline{x} + \lambda(\overline{x} - x_{(P+1)}),$$

where λ is a tuning parameter kept fixed, typically $\lambda = 1$.

If x^r is better than the second-worst but not the best one we have at this stage — i.e. $f(x_{(1)}) \leq f(x^r) \leq f(x_{(P)})$ — then we replace$x_{(P+1)}$ with x^r and go to step 1.

If x^r is the best we have seen so far, go to step 4.

If x^r is not even better than the second-worst, go to step 5.

If x^r is worse than the worst point, go to step 6.

4 (expansion). If the reflected point is better than anything we currently have — $f(x^r) < f(x_{(1)})$ — then we compute the expanded point,

$$x^e = \overline{x} + \gamma(\overline{x} - x_{(P+1)}).$$

Typically, $\gamma = 2$. Note that both x^r and x^e are on the 1-dimensional line through $x_{(P+1)}$ and $\overline{x}$. Replace the worst point ($x_{(P+1)}$) by whichever of x^r and x^e gives the best function value. The expansion is sometimes referred to as a *greedy minimization approach*, where the indication that there might be improvements in the direction of x^r is exploited by taking further steps in that direction.

5 (contraction). In this case $f(x^r) \geq f(x_{(P)})$ so that the reflected point is no better than the previous second-worst. The contraction step is performed using x^r if this is better than $x_{(P+1)}$ (*outside contraction*) or $x_{(P+1)}$ if this is better than x^r (*inside contraction*):

(outside contraction) If $f(x_{(P)}) \leq f(x^r) < f(x_{(P+1)})$, compute

$$x^c = \overline{x} + \beta(x^r - \overline{x}),$$

where e.g. $\beta = \frac{1}{2}$. If x^c is better than x^r, replace $x_{(P+1)}$ with x^c and go to step 1. If x^c is not better than x^r, go to step 6.

(inside contraction) If $f(x^r) \geq f(x_{(P+1)})$, compute

$$x^c = \overline{x} + \beta(x_{(P+1)} - \overline{x}).$$

If x^c is better than $x_{(P+1)}$, accept it and go to step 1. Otherwise go to step 6.

6 (shrink). This steps shrinks all the sides of the simplex in the direction of the best point so far by setting

$$x_{(p)} := x_{(1)} + \delta(x_{(p)} - x_{(1)}), \quad p \neq 1.$$

Typically, $\delta = \frac{1}{2}$. In other words, all points except for the best ($x_{(1)}$) are moved half way towards the best point. After this step, go to step 1.

The algorithm will terminate when either the change in x or $f(x)$ becomes sufficiently small. This is computed as

$$\begin{aligned} &\text{tolerance measure in } x: \quad \tfrac{\|x_{g+1} - x_g\|}{\|x_g\|}, \\ &\text{tolerance measure in } f: \quad \tfrac{|f(x_{g+1}) - f(x_g)|}{|f(x_g)|}. \end{aligned}$$

Matlab typically uses the "infinity norm" for vectors, $\|x\|_\infty \equiv \max_k |x_k|$.

4 Matlab Example: The Rosenbrock Function

In this section, we will consider the minimization of the Rosenbrock function and compare how well `fminunc` (gradient-based) and `fminsearch` (gradient-free) do at finding the global minimum.

The function is defined by

$$f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2.$$

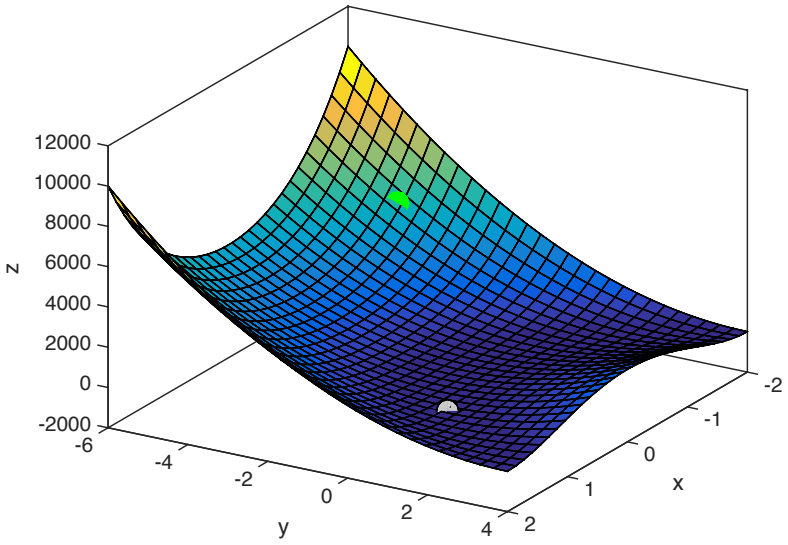
The function is shown in Figure 4 along with the global minimum at $x = (1, 1)$ and the starting value we will be using at $x_0 = (-1.5, -4)$. The gradient vector of partial derivatives is

$$\begin{aligned} \nabla f(x_1, x_2) &= \left(\tfrac{\partial f}{\partial x_1}, \quad \tfrac{\partial f}{\partial x_2}\right) \\ &= \left(-400(x_2 - x_1^2)x_1 - 2(1 - x_1), \quad 200(x_2 - x_1^2)\right). \end{aligned}$$

The Matlab code for the function and its gradient is given below:

```
function [f,g] = rosenbrock(x)
% Returns the Rosenbrock function with gradients.
% Note: x should have two elements.
f = 100*(x(2) - x(1)^2)^2 + (1-x(1))^2;
if nargout > 1 % Computed if the gradient is required
```

Figure 4: The Rosenbrock Function




```
6       g(1) = -400*(x(2)-x(1)^2)*x(1)-2*(1-x(1));
7       g(2) =  200*(x(2)-x(1)^2);
8   end
```

We save this file as `rosenbrock.m`. Note that if the function is asked for more than one output (`nargout>1`), it will return the variable `g`, which will be two-dimensional (since the gradient should have two entries, one for each partial derivative).

4.1 BFGS

We will first minimize the function using a gradient-based solver, `fminunc`. To do this, we must first set the optimization options.

```
1  opt = optimoptions(@fminunc,...
2      'Display','iter',... % shows output at each iteration step
3      'gradobj','on',... % use analytic gradients
4      'Algorithm','quasi-newton',...
5      'HessUpdate','bfgs',... % set the Hessian-update to BFGS
6      'TolFun',1e-08,... % main tolerance (gradients)
7      'TolX',1e-08, ...  % x-change tolerance
8      'MaxIter',300,... % max iterations
9      'MaxFunEvals',500,... % max function evaluations
10     'DerivativeCheck','on' ... % check our analytic gradients
11     );
```

We have specified quite strict stopping criteria, namely tolerances of 10^{-8}. It may not always be possible to get the gradients to be so small, in particular if there is numerical noise in the function evaluation and numerical gradients are being used. We are now ready to specify the the initial point and start the optimizer.

```
x0 = [-1.5;-4];
[xhat,fhat,flag,out,ghat,hhat] = fminunc(@rosenbrock,x0,opt);
```

This tells Matlab to start the optimization at the point $x_0 = (-1.5, -4)$ using the specified options. Note that the "`@`" indicates to Matlab that `rosenbrock` is a *function handle* object and not a variable. The output from running this is:

```
                                                         First-order
 Iteration  Func-count       f(x)        Step-size       optimality
     0           1           3912.5                      3.76e+03
     1           2          1536.63    0.000266312            786
     2           3          1135.01              1            673
     3           4          650.897              1            510
     4           5          309.937              1            377
     5           6          60.3901              1            244
     6           7          2.43146              1           55.4
     7           8        0.0148755              1           3.02
     8           9       0.00703328              1           0.18
     9          11       0.00693671             10          0.515
    10          13       0.00530386             10          0.625
    11          15      0.000918213            0.5          0.549
    12          16      0.000408093              1           0.61
    13          17      2.15428e-05              1         0.0491
    14          18      4.86863e-07              1         0.0251
    15          19      5.33201e-09              1        0.00221
    16          20      2.83783e-13              1       1.76e-05

Local minimum found.

Optimization completed because the size of the gradient is less than
the selected value of the function tolerance.

<stopping criteria details>
```

The first thing we note is that `fminunc` terminated due to the gradients being smaller than the tolerance; this indicates that we have indeed found a stationary point. It took 16 iterations and 20 function evaluations to get to the stationary point. Matlab also indicates this to us by saying "`Local minimum found`". Later, we shall see examples of termination due

to other criteria, where it says "`Local minimum possible`". The first and second columns indicate the iteration and function evaluation count. The column `f(x)` indicates the value of the objective function and we see that the function value at termination is `2.8e-13`, which is very close to 0 (the value at $f(1,1)$). The column `Step-size` indicates that we are using a line-search algorithm and shows the size of λ. We see that the first step was small and that in iterations 9 and 10, a large step-size was used (in these steps, the optimizer used two function evaluations each, indicating that it was searching along the line). In particular, $\lambda = 10$ was used, indicating that Matlab was greedily moving further along the search direction than indicated by the Hessian. In iteration 11, it took a smaller step ($\lambda = 0.5$), so maybe it encountered an increase in f for $\lambda = 1$. The final column, `First-order optimality`, indicates that the infinity-norm of the gradient at the termination value was $1.76 \cdot 10^{-5}$. If we click on `<stopping criteria details>` (which is a link in Matlab), we are shown further details.

```
1 Optimization completed: The first-order optimality measure, 4.682554e-09, is less
2 than options.TolFun = 1.000000e-08.
3
4 Optimization Metric                                          Options
5 relative norm(gradient) =   4.68e-09                TolFun =   1e-08 (selected)
```

This reminds us that the first-order optimality measure is a *relative* gradient. The number is computed as

$$\texttt{relative}\,\texttt{norm}(\texttt{gradient}) = \frac{\|\nabla f(x^*)\|_\infty}{\|\nabla f(x_0)\|_\infty},$$

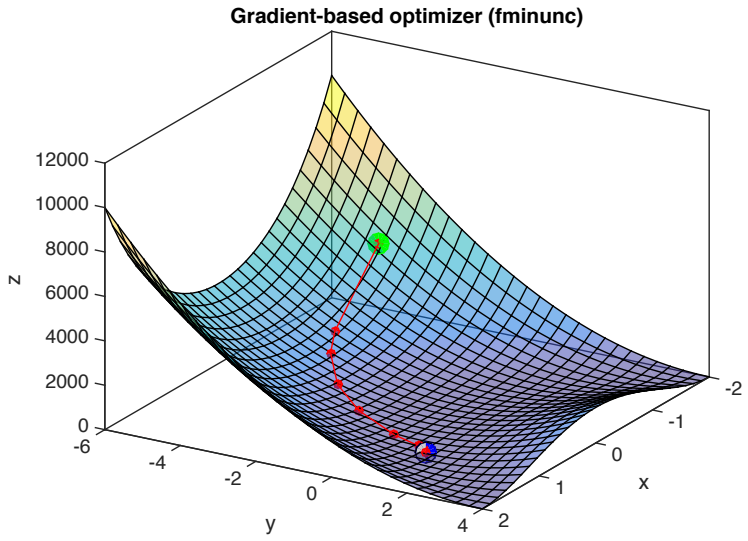
where x^* is the found minimizer. That is, if we run

```
1 [f0,g0] = rosenbrock(x0);
2 norm(ghat,inf) / norm(g0,inf)
```

then we get the reported relative norm of `4.6838e-09`. Note that this implies that Matlab is solving a problem that is scaled relative to the initial value. In other words, for a fixed `opt.TolFun` of `1e-08`, it will take more iterations if we start it again from the minimizer, `xhat`. From the output, we see that the *actual* (non-relative) first-order optimality measure (the highest absolute value of the two entries in the gradient) is `1.76e-05`. In other words, we are probably very close. Nevertheless, one should always pay attention to these details after the optimizer has converged.

Figure5 shows the steps taken by `fminunc` in minimizing the function. The convergence to the global minimum is quite fast and occurs very smoothly.

Figure 5: Gradient-based Optimizer (`fminunc`) minimizing the Rosenbrock Function



4.2 Steepest Descent

Let us try minimizing the function using the steepest descent algorithm. To do this, we need to set the option `HessUpdate` to `'steepdesc'` instead of `'bfgs'` in the example above. The optimization procedure finds the global minimum but it takes 56,649 function evaluations to do so, compared to just 20 function evaluations for the BFGS algorithm. We also see that while the step size for the BFGS algorithm was 1 in all but 4 of the iterations, it changes in every single iteration for the steepest descent algorithm. This is because the optimizer is using the line search procedure to figure out how far to go along the direction of the gradient, whereas the BFGS procedure uses the information in the Hessian to judge how far to go.

```
                                                          First-order
 Iteration  Func-count       f(x)        Step-size       optimality
     0           3           3912.5                      3.76e+03
     1           6           1536.63    0.000266312           786
     2          27           1026.16     0.00194496       1.32e+03
     3          51           253.655     0.00100537            317
     4          69           27.3169     0.00827851            269
     5          93         0.0095388    0.000703912          0.676

...

  4727       56616       2.81842e-09          0.001       4.69e-05
  4728       56622        2.2199e-09       0.469188       0.000854
```

```
   4729       56634      1.78798e-09          0.001       3.81e-05
   4730       56637      1.76329e-09              1        0.00141
   4731       56649       5.5695e-10          0.001       2.36e-05

Local minimum found.

Optimization completed because the size of the gradient is less than
the selected value of the optimality tolerance.

<stopping criteria details>
```

4.3 Gradient-free Optimization

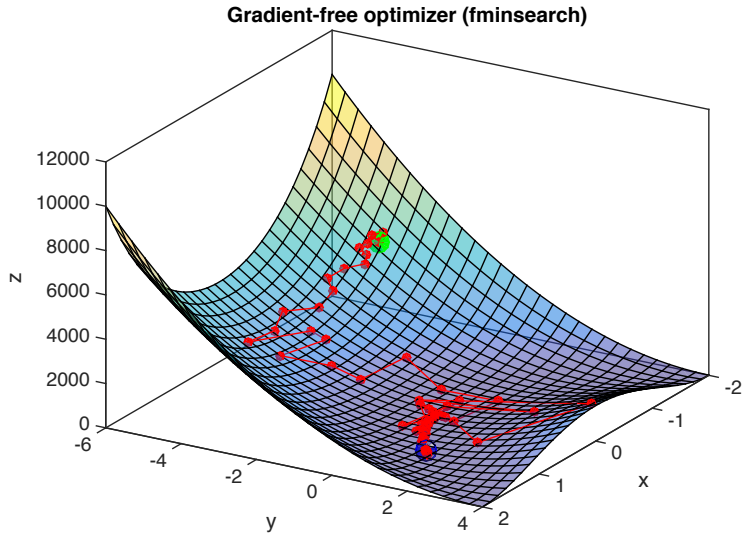
If we instead want to minimize the function using Nelder-Mead (`fminsearch`), the required code is

```
x0 = [-1.5;-4];
opt = optimset('Display','iter',...
    'TolX',1e-08,...
    'TolFun',1e-08,...
    'MaxIter',500,...
    'MaxFunEvals',1000);
xhat = fminsearch(@(x)rosenbrock(x),x0,opt);
```

The output from the function is very long since it takes 100 iterations and 194 evaluations until convergence so we will consider only an extract of it.

```

 Iteration   Func-count     min f(x)         Procedure
      0            1           3912.5
      1            3           3912.5         initial simplex
      2            5          3754.02         expand
      3            7          3226.45         expand
      4            9          2923.97         expand
      5           11          2160.55         expand
      6           12          2160.55         reflect
      7           14          2004.75         reflect
      8           16          1390.74         expand

...

     96          186      4.11134e-17         contract outside
     97          188      1.27001e-17         contract inside
     98          190      1.27001e-17         contract inside
```

Figure 6: Gradient-free Optimizer (`fminsearch`) minimizing the Rosenbrock Function




```
18      99          192       9.32149e-18         contract inside
19     100          194       6.88373e-18         contract outside
20
21  Optimization terminated:
22   the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-08
23   and F(X) satisfies the convergence criteria using OPTIONS.TolFun of 1.000000e-08
```

We see that the final point satisfies both the convergence criterion for the change in x and the change in $f(x)$. Figure 6 shows the steps taken towards the minimum point. We see that the optimizer is taking many more steps but eventually gets to the true minimum. Moreover, with the chosen tolerances, `fminsearch` gets below 10^{-9} in maximum absolute distance from $(1, 1)$ whereas `fminunc` only gets to 10^{-6}. This is because `fminunc` uses the initial gradients as the relative termination measure; we could get it much closer if we wished. But it illustrates that `fminsearch` can get very precise as well given enough iterations.

4.4 A More Difficult Example: Illustrating the Effect of Noise

In this section, we will consider an example where we add noise to the function evaluation. This results in the gradient-based optimizer failing miserably when it uses numerical gradients and not working very well even when analytic gradients are used. The gradient-free optimizer is much more robust to this type of noise.

Suppose that we add some noise to the Rosenbrock function in the form of a random

normal variable with a standard deviation of 10^{-4}. That is

$$\tilde{f}(x_1, x_2) = f(x_1, x_2) + 10^{-4}\eta, \quad \eta \sim \mathcal{N}(0, 1).$$

In code, we write this as

```
function [f,g] = rosenbrock(x)
f = 100*(x(2) - x(1)^2)^2 + (1-x(1))^2 + 1e-04*randn(1,1);
if nargout > 1 % gradients are noise-free
    g(1) = -400*(x(2)-x(1)^2)*x(1)-2*(1-x(1));
    g(2) =  200*(x(2)-x(1)^2);
end
```

We start `fminunc` with the code

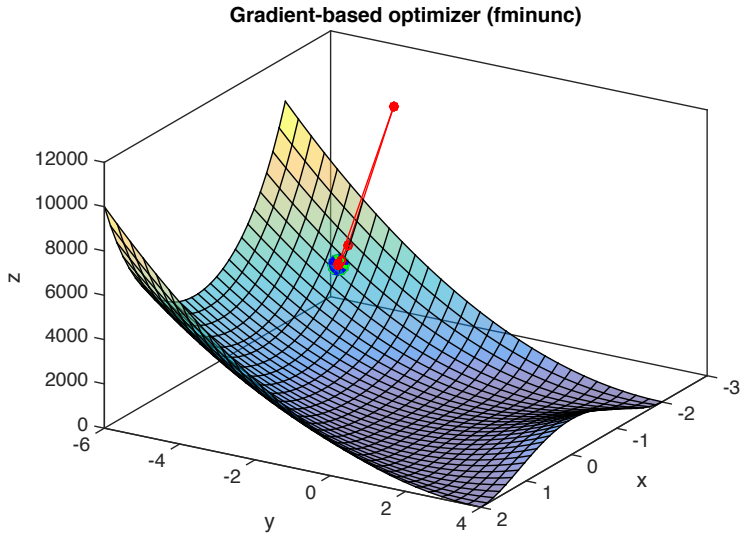
```
x0 = [-1.5;-4];
opt = optimoptions(@fminunc,...
    'Display','iter',...
    'gradobj','off',...
    'Algorithm','quasi-newton',...
    );
rng(1); % initialize random number generator
[xhat,fhat,flag,out,ghat,hhat] = fminunc(@rosenbrock,x0,opt);
```

Note that we initialize the random number generator to show the same path every time (since there is now a random element in f). We can change the seed (`1` above) to see different paths. In this simulation, the output is

```

                                                         First-order
 Iteration  Func-count       f(x)        Step-size       optimality
     0           3           3912.5                      7.06e+03
     1          48           3912.5    6.73466e-15       4.45e+03

Local minimum possible.

fminunc stopped because the size of the current step is less than
the selected value of the step size tolerance.

<stopping criteria details>
```

When Matlab says "`Local minimum possible`", we should always be aware of potential problems. The exit message indicates that the line search has failed. Figure 7 shows what has happened; the optimizer starts off immediately in the wrong direction, tries to line-search

Figure 7: Gradient-based Optimizer (`fminunc`) Failing Due to Stochastic Noise



to get an improvement but finds none and eventually terminates having taken 48 function evaluations down to a step size so small ($6.8 \cdot 10^{-15}$) that it gives up.

What went wrong? The reason is that the numerical gradients will be way off. When `fminunc` takes a small step of $h = \sqrt{\epsilon} \cong 10^{-8}$, it gets a new random shock on the order of 10^{-4}, which means that it will get a completely wrong indication of the local slope. If instead we set `gradobj` to `on`, Matlab uses the analytic gradients, which helps, but the optimizer converges to $x^* = (0.92, 0.84) \neq (1, 1)$, which is better but still not at the global optimum.

On the other hand, `fminsearch` does not converge even with 5000 iterations. However, it gets to the final point $x^* = (0.998, 0.996)$, which is very close to $(1, 1)$ considerting that the noise is on the order of 0.0001. After 834 iterations, it reaches a function value of $3.5 \cdot 10^{-4}$ and then it does not change for the next 4,166 iterations.

```
1   Iteration   Func-count     min f(x)         Procedure
2       0            1           3912.5
3       1            3           3912.5         initial simplex
4       2            5          3754.02         expand
5       3            7           3226.45        expand
6   ...
7    4999        13144     -0.000350547         shrink
8    5000        13148     -0.000350547         shrink
9
10  Exiting: Maximum number of iterations has been exceeded
11           - increase MaxIter option.
12           Current function value: -0.000351
```

5 Troubleshooting

In this section, we will consider a number of symptoms, some likely causes and ideas for solutions.

Problem	**Possible solutions**
[anything]	Try debugging your code. See if you can simplify your problem to something where the solution is trivial/easier; too many bugs are simpler than you might imagine. Shut down parts of the model you do not need. Work on simulated data if at all possible. Try using Matlab's `keyboard` function for debugging functions. See Section 5.1.
Noise in the criterion function	**Roundoff errors:** Look for things in your code that might become really small or large. For example, if you could be taking `log` of something too close to zero or `exp` of a large number (e.g., `exp(800) = inf`). Also functions like `normpdf` can cause roundoff error for inputs far from zero. **Simulation/stochastic problems:** If you are using *simulation* methods (if there is any random draws in your evaluation), make sure your seed is fixed and does not change every time you evaluate the criterion function. Try

Unable to find good starting values / function undefined at initial point	If you cannot think of a good set of starting values, it will typically mainly be a few of the parameters. In that case, try doing a *grid search*. I.e. define a range of points (e.g. 10 points from 0 to 1000 below) and then loop through the points and print the function value of your function, say `myFunc(.)`,
	`xx = linspace(0,1000,10);`
	`for i=1:numel(xx);`
	`  x = x0; % values of the fixed parameters`
	`  x(k) = xx(i); % change only x_k`
	`  fprintf('Fun value at x=%5.3g: %5.3g.\n',...`
	`  xx(i),myFunc(x));`
	`end;`
	Using similar code, you can also hold fixed some of the parameters and search over only one of the parameters.

Problem	Possible solutions
Function evaluation is very slow	There are many potential reasons why evaluation might be slow. Matlab has a tool called the `Profiler` (the button is called "Run and Time" under the "Editor" tab). This will run a script and time for you which part of your code takes time with nice coloring and indications of seconds spent in each part of the code. This tool is surprisingly useful for finding out which part of your code is bottlenecking. Some general advise for speeding up Matlab code is given in Section 5.2
Max iterations reached without convergence	If possible try to increase `MaxIter` and `MaxFunEvals` to see if this helps. If the function value is unchanged for many many iterations, you could have numerical noise in your criterion function (see previous table).
Step size too small (line search fails)	The gradients or the Hessian could be wrong or you could be in a local area of non-convexity. Try using `fminsearch`.

5.1 Debugging Matlab Code

For debugging Matlab code, practice makes perfect. As a first step, one should of course follow the error messages in Matlab.

Keyboard: Try using the `keyboard` function if the error occurs in a nested function. To do this, insert a line just before the line where the error occurs with the statement "`keyboard;`". When you then run the code, Matlab will stop at the line (as indicated by a green arrow to the left of it). The work space will now look exactly as it does when Matlab has reached this point. In the `Editor`-fan, the buttons have changed because you are now in debug-mode. You can exit debug mode at any point by pressing `dbquit;` in the terminal or the red button labelled `Quit Debugging`. You can now run the function line-by-line by pressing the `Step`-button. You can also print out the variables that are in memory or run parts of the line that causes the error.
This approach can be very useful for discovering errors in the dimensions of the variables or for fixing syntax errors or incorrect parentheses.

Simplifying: The best advice for debugging is to simplify the code; try to see how simple you can make the setting and still replicate the bug. Shut off as many parts of the model as you possibly can and comment out parts of the code. Then, when you get to a working version, add them back in one at the time.

Narrowing down the cause: Try to be systematic about how you find the cause of your bug; think of a possible problem that could be causing the symptoms you are seeing

and then think of a way of testing if that is correct.

Data read incorrectly: Try to work on simulated data and create a very simple data generating process where you can narrow this down. Maybe work only with $N = 2$ and $T = 2$ and use `keyboard` to see what is in the data matrices in the very core of the function where your criterion function is computed.

Parameters enter incorrectly: If you suspect a bug where, for example, the variance term enters incorrectly. Then think about intuitively what the effect should be of increasing the variance term; in most cases, it should mean that the predicted values of the model should get closer to each other (the variance washes out all the differences). Then check if this happens.

Plotting over a grid: Often, it might make sense to form a grid over one or more parameters and calculate the objective value at each of these points and then plot it. This can sometimes tell a lot about what can be wrong.

Randomness: If you think there is randomness in your function, evaluate the function twice at the same point to see if it returns precisely the same value.

Numerical noise: If you think there is numerical noise in your function, try doing a forward and a backwards finite difference (derivative-approximation). If the function is well-behaved, the two should give approximately the same slope.

5.2 Speeding Up Matlab Code

As mentioned in the table, the first thing you should do is to time your code using the `Profiler` to find our exactly what is bottlenecking. It is an absolutely essential first step to use the `Profiler` as your might otherwise spend ages trying to get speed improvements at a step, which did not take much time in the first place. Apart from this, Matlab gives tips on improvements to your code in the right-hand side of the code editor, which you should of course try to follow where possible. Below we will consider a few concrete examples.

Pre-computation. Consider if there is something in your function evaluation, which you are re-calculating at each step but does not change. This might include interacting variables instead of doing the multiplication at each step. The

Loops. Matlab is notoriously slow with for-loops and while-loops even though this is by many considered to be a good way of coding (and in some languages the only one). If possible, you should try to replace such loops with vectorized operations instead. For example,

```
1 % Slow way
2 mySum = 0;
```

```
for i=1:numel(X);
    mySum = mySum + X(i);
end;
% Fast way
mySum = sum(X(:));
```

Sometimes, vectorizing can be very hard but often it is possible.

Indexing. You should generally try to work with indexing.

```
% Very slow way
for i=1:numel(X);
    if X(i)>0;
        f(i)=funcNum1(X(i));
    else X(i)<=0;
        f(i)=funcNum2(X(i));
    end;
end;
% Fast way
idxPos = X>0;
idxNeg = x<=0;
f(idxPos) = funcNum1(X(idxPos));
f(idxNeg) = funcNum2(X(idxNeg));
```

Similarly, you may often need to pick out for example the first year for each observation. Then it is useful to have a matrix of 0/1's where 1 indicates that it is the first year for an individual. You can either work with index matrices that are binary (0/1 for each observation) or integer-valued (each number corresponding to a row-number in your data matrix). This can really speed up your code substantially.

Pre-allocating. If you are using an index matrix very often and it is very large, then sometimes it will make sense to give it as an input to your objective function rather than creating it again at every iteration.

Repmat. Even though it is a convenient function, `repmat` can be very slow and it has a faster alternative method. This is relevant in particular when doing elementwise multiplication, which one often may need to do when doing for example simulated maximum likelihood or conditional logit.

```
X = rand(100,10);
fact = rand(1,10);
% Slow way
productMatrix = X .* repmat(fact,100,1);
```

```
% Fast way
productMatrix = X .* fact(ones(100,1),:);
```

Parallelization. Matlab can work on multiple CPUs if your computer has them. To use this, type `matlabpool open N`, where `N` is the number of cores you wish to use (setting `N` higher than your computer's number of processors will not help you further). This will allow you to for example use the `parfor` loop, which can sometimes speed up your code. In practice, I have personally found that the gain here rarely is very big. The topic of parallel computing is beyond the scope of this note but there are plenty of resources online.

Using `c` code. The programming language, `c`, is an extremely powerful language that can achieve incredible speeds for complicated programming tasks. However, it takes considerable experience to become good at coding `c`, and often you will spend more time debugging than you would expect. That being said, it can be an excellent tool. There are two options for working with `c` code in Matlab; the Matlab `c` code generator and the `Mex` interface. Before going to `c`, consider if there is some tuning or precision parameter that your could turn down instead to speed up your code.

Code generator. If your code is simple enough, Matlab can understand it and create `c` code that can do the computations. This can sometimes speed up your calculations substantially without requiring too much human time input coding and debugging. Google it to find a nice tutorial.

`Mex`. Matlab is written in `c` and the `mex` interface allows you to interact with Matlab's structures directly in `c`. This can be extraordinarily time-consuming and the learning curve is extremely steep but for some projects, e.g. structural estimation, the final speedup may be a factor of several hundred so it can be worth it. Again, plenty of tutorials and resources are available online.