AM 205: lecture 17

- Assignment 4 posted
- Midterm will be uploaded at 5 PM on Thursday November 13. Due at 5 PM on Friday November 14.
- Last time: introduction to optimization
- Today: scalar and vector optimization

Fixed-Point Iteration

Recall that if $g \in C^1[a, b]$, we can obtain a Lipschitz constant based on g':

$$L = \max_{\theta \in (a,b)} |g'(\theta)|$$

We now use this results to show that if $|g'(\alpha)| < 1$, then there is a neighborhood of α on which g is a contraction

This tells us that we can verify convergence of a fixed point iteration by checking the gradient of g

Fixed-Point Iteration

By continuity of g' (and hence continuity of $|g'|$), for any $\epsilon > 0$ $\exists \delta > 0$ such that for $x \in (\alpha - \delta, \alpha + \delta)$:

$$\big|\,|g'(x)| - |g'(\alpha)|\,\big| \leq \epsilon \implies \max_{x \in (\alpha-\delta,\alpha+\delta)} |g'(x)| \leq |g'(\alpha)| + \epsilon$$

Suppose $|g'(\alpha)| < 1$ and set $\epsilon = \frac{1}{2}(1 - |g'(\alpha)|)$, then there is a neighborhood on which g is Lipschitz with $L = \frac{1}{2}(1 + |g'(\alpha)|)$

Then $L < 1$ and hence g is a contraction in a neighborhood of α

Fixed-Point Iteration

Furthermore, as $k \to \infty$,

$$\frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} = \frac{|g(x_k) - g(\alpha)|}{|x_k - \alpha|} \to |g'(\alpha)|,$$

Hence, asymptotically, error decreases by a factor of $|g'(\alpha)|$ each iteration

Fixed-Point Iteration

We say that an iteration converges linearly if, for some $\mu \in (0, 1)$,

$$\lim_{k\to\infty} \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} = \mu$$

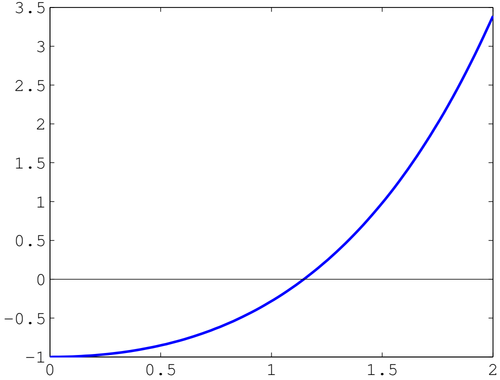
An iteration converges superlinearly if

$$\lim_{k\to\infty} \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} = 0$$

Fixed-Point Iteration

We can use these ideas to construct practical fixed-point iterations for solving $f(x) = 0$

e.g. suppose $f(x) = e^x - x - 2$



From the plot, it looks like there's a root at $x \approx 1.15$

Fixed-Point Iteration

$f(x) = 0$ is equivalent to $x = \log(x + 2)$, hence we seek a fixed point of the iteration

$$x_{k+1} = \log(x_k + 2), \quad k = 0, 1, 2, \ldots$$

Here $g(x) \equiv \log(x + 2)$, and $g'(x) = 1/(x + 2) < 1$ for all $x > -1$, hence fixed point iteration will converge for $x_0 > -1$

Hence we should get linear convergence with factor approx. $g'(1.15) = 1/(1.15 + 2) \approx 0.32$

Fixed-Point Iteration

An alternative fixed-point iteration is to set

$$x_{k+1} = e^{x_k} - 2, \quad k = 0, 1, 2, \ldots$$

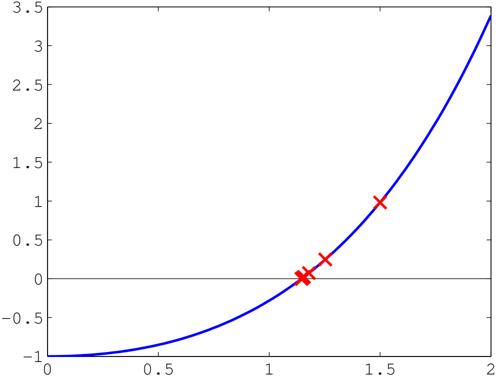
Therefore $g(x) \equiv e^x - 2$, and $g'(x) = e^x$

Hence $|g'(\alpha)| > 1$, so we can't guarantee convergence

(And, in fact, the iteration diverges...)

Fixed-Point Iteration

Python demo: Comparison of the two iterations



Newton's Method

Constructing fixed-point iterations can require some ingenuity

Need to rewrite $f(x) = 0$ in a form $x = g(x)$, with appropriate properties on g

To obtain a more generally applicable iterative method, let us consider the following fixed-point iteration

$$x_{k+1} = x_k - \lambda(x_k)f(x_k), \quad k = 0, 1, 2, \ldots$$

corresponding to $g(x) = x - \lambda(x)f(x)$, for some function λ

A fixed point α of g yields a solution to $f(\alpha) = 0$ (except possibly when $\lambda(\alpha) = 0$), which is what we're trying to achieve!

Newton's Method

Recall that the asymptotic convergence rate is dictated by $|g'(\alpha)|$, so we'd like to have $|g'(\alpha)| = 0$ to get superlinear convergence

Suppose (as stated above) that $f(\alpha) = 0$, then

$$g'(\alpha) = 1 - \lambda'(\alpha)f(\alpha) - \lambda(\alpha)f'(\alpha) = 1 - \lambda(\alpha)f'(\alpha)$$

Hence to satisfy $g'(\alpha) = 0$ we choose $\lambda(x) \equiv 1/f'(x)$ to get Newton's method:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k = 0, 1, 2, \ldots$$

Newton's Method

Based on fixed-point iteration theory, Newton's method is convergent since $|g'(\alpha)| = 0 < 1$

However, we need a different argument to understand the superlinear convergence rate properly

To do this, we use a Taylor expansion for $f(\alpha)$ about $f(x_k)$:

$$0 = f(\alpha) = f(x_k) + (\alpha - x_k)f'(x_k) + \frac{(\alpha - x_k)^2}{2}f''(\theta_k)$$

for some $\theta_k \in (\alpha, x_k)$

Newton's Method

Dividing through by $f'(x_k)$ gives

$$\left(x_k - \frac{f(x_k)}{f'(x_k)}\right) - \alpha = \frac{f''(\theta_k)}{2f'(x_k)}(x_k - \alpha)^2,$$

or

$$x_{k+1} - \alpha = \frac{f''(\theta_k)}{2f'(x_k)}(x_k - \alpha)^2,$$

Hence, roughly speaking, the error at iteration $k+1$ is the square of the error at each iteration k

This is referred to as quadratic convergence, which is very rapid!

Key point: Once again we need to be sufficiently close to α to get quadratic convergence (result relied on Taylor expansion near α)

Secant Method

An alternative to Newton's method is to approximate $f'(x_k)$ using the finite difference

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

Substituting this into the iteration leads to the secant method

$$x_{k+1} = x_k - f(x_k)\left(\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}\right), \quad k = 1, 2, 3, \ldots$$

The main advantages of secant are:

- does not require us to determine $f'(x)$ analytically
- requires only one extra function evaluation, $f(x_k)$, per iteration (Newton's method also requires $f'(x_k)$)

Secant Method

As one may expect, secant converges faster than a fixed-point iteration, but slower than Newton's method

In fact, it can be shown that for the secant method, we have

$$\lim_{k\to\infty} \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|^q} = \mu$$

where μ is a positive constant and $q \approx 1.6$

Python demo: Newton's method versus secant method for $f(x) = e^x - x - 2 = 0$

Multivariate Case

Systems of Nonlinear Equations

We now consider fixed-point iterations and Newton's method for systems of nonlinear equations

We suppose that $F : \mathbb{R}^n \to \mathbb{R}^n$, $n > 1$, and we seek a root $\alpha \in \mathbb{R}^n$ such that $F(\alpha) = 0$

In component form, this is equivalent to

$$\begin{aligned} F_1(\alpha) &= 0 \\ F_2(\alpha) &= 0 \\ &\vdots \\ F_n(\alpha) &= 0 \end{aligned}$$

Fixed-Point Iteration

For a fixed-point iteration, we again seek to rewrite $F(x) = 0$ as $x = G(x)$ to obtain:

$$x_{k+1} = G(x_k)$$

The convergence proof is the same as in the scalar case, if we replace $|\cdot|$ with $\|\cdot\|$

i.e. if $\|G(x) - G(y)\| \leq L\|x - y\|$, then $\|x_k - \alpha\| \leq L^k \|x_0 - \alpha\|$

Hence, as before, if G is a contraction it will converge to a fixed point α

Fixed-Point Iteration

Recall that we define the Jacobian matrix, $J_G \in \mathbb{R}^{n\times n}$, to be

$$(J_G)_{ij} = \frac{\partial G_i}{\partial x_j}, \quad i,j = 1,\ldots,n$$

If $\|J_g(\alpha)\|_\infty < 1$, then there is some neighborhood of α for which the fixed-point iteration converges to α

The proof of this is a natural extension of the corresponding scalar result

Fixed-Point Iteration

Once again, we can employ a fixed point iteration to solve $F(x) = 0$

e.g. consider

$$\begin{aligned} x_1^2 + x_2^2 - 1 &= 0 \\ 5x_1^2 + 21x_2^2 - 9 &= 0 \end{aligned}$$

This can be rearranged to $x_1 = \sqrt{1 - x_2^2}$, $x_2 = \sqrt{(9 - 5x_1^2)/21}$

Fixed-Point Iteration

Hence, we define

$$G_1(x_1, x_2) \equiv \sqrt{1 - x_2^2}, \;\; G_2(x_1, x_2) \equiv \sqrt{(9 - 5x_1^2)/21}$$

Python Example: This yields a convergent iterative method

Newton's Method

As in the one-dimensional case, Newton's method is generally more useful than a standard fixed-point iteration

The natural generalization of Newton's method is

$$x_{k+1} = x_k - J_F(x_k)^{-1} F(x_k), \quad k = 0, 1, 2, \ldots$$

Note that to put Newton's method in the standard form for a linear system, we write

$$J_F(x_k) \Delta x_k = -F(x_k), \quad k = 0, 1, 2, \ldots,$$

where $\Delta x_k \equiv x_{k+1} - x_k$

Newton's Method

Once again, if x_0 is sufficiently close to α, then Newton's method converges quadratically — we sketch the proof below

This result again relies on Taylor's Theorem

Hence we first consider how to generalize the familiar one-dimensional Taylor's Theorem to $\mathbb{R}^n$

First, we consider the case for $F : \mathbb{R}^n \to \mathbb{R}$

Multivariate Taylor Theorem

Let $\phi(s) \equiv F(x + s\delta)$, then one-dimensional Taylor Theorem yields

$$\phi(1) = \phi(0) + \sum_{\ell=1}^{k} \frac{\phi^{(\ell)}(0)}{\ell!} + \phi^{(k+1)}(\eta), \quad \eta \in (0,1),$$

Also, we have

$$\begin{aligned}
\phi(0) &= F(x) \\
\phi(1) &= F(x+\delta) \\
\phi'(s) &= \frac{\partial F(x+s\delta)}{\partial x_1}\delta_1 + \frac{\partial F(x+s\delta)}{\partial x_2}\delta_2 + \cdots + \frac{\partial F(x+s\delta)}{\partial x_n}\delta_n \\
\phi''(s) &= \frac{\partial^2 F(x+s\delta)}{\partial x_1^2}\delta_1^2 + \cdots + \frac{\partial^2 F(x+s\delta)}{\partial x_1 x_n}\delta_1\delta_n + \cdots + \\
&\quad \frac{\partial^2 F(x+s\delta)}{\partial x_1 \partial x_n}\delta_1\delta_n + \cdots + \frac{\partial^2 F(x+s\delta)}{\partial x_n^2}\delta_n^2 \\
&\vdots
\end{aligned}$$

Multivariate Taylor Theorem

Hence, we have

$$F(x+\delta) = F(x) + \sum_{\ell=1}^{k} \frac{U_\ell(\delta)}{\ell!} + E_k,$$

where

$$U_\ell(x) \equiv \left[\left(\frac{\partial}{\partial x_1}\delta_1 + \cdots + \frac{\partial}{\partial x_n}\delta_n\right)^\ell F\right](x), \quad \ell = 1, 2, \ldots, k,$$

and

$$E_k \equiv U_{k+1}(x+\eta\delta), \quad \eta \in (0,1)$$

Multivariate Taylor Theorem

Let A be an upper bound on the abs. values of all derivatives of order $k+1$, then

$$
\begin{aligned}
|E_k| &\leq \frac{1}{(k+1)!}\left|(A,\ldots,A)^T\left(\|\delta\|_\infty^{k+1},\ldots,\|\delta\|_\infty^{k+1}\right)\right| \\
&= \frac{1}{(k+1)!}A\|\delta\|_\infty^{k+1}\left|(1,\ldots,1)^T(1,\ldots,1)\right| \\
&= \frac{n^{k+1}}{(k+1)!}A\|\delta\|_\infty^{k+1}
\end{aligned}
$$

where the last line follows from the fact that there are n^{k+1} terms in the inner product (*i.e.* there are n^{k+1} derivatives of order $k+1$)

Multivariate Taylor Theorem

We shall only need an expansion up to first order terms for analysis of Newton's method

From our expression above, we can write first order Taylor expansion succinctly as:

$$F(x + \delta) = F(x) + \nabla F(x)^T \delta + E_1$$

Multivariate Taylor Theorem

For $F : \mathbb{R}^n \to \mathbb{R}^n$, Taylor expansion follows by developing a Taylor expansion for each F_i, hence

$$F_i(x + \delta) = F_i(x) + \nabla F_i(x)^T \delta + E_{i,1}$$

so that for $F : \mathbb{R}^n \to \mathbb{R}^n$ we have

$$F(x + \delta) = F(x) + J_F(x)\delta + E_F$$

where $\|E_F\|_\infty \leq \max_{1 \leq i \leq n} |E_{i,1}| \leq \frac{1}{2} n^2 \left(\max_{1 \leq i,j,\ell \leq n} \left| \frac{\partial^2 F_i}{\partial x_j \partial x_\ell} \right| \right) \|\delta\|_\infty^2$

Newton's Method

We now return to Newton's method

We have

$$0 = F(\alpha) = F(x_k) + J_F(x_k)\,[\alpha - x_k] + E_F$$

so that

$$x_k - \alpha = [J_F(x_k)]^{-1} F(x_k) + [J_F(x_k)]^{-1} E_F$$

Newton's Method

Also, the Newton iteration itself can be rewritten as

$$J_F(x_k)\,[x_{k+1}-\alpha] = J_F(x_k)\,[x_k-\alpha] - F(x_k)$$

Hence, we obtain:

$$x_{k+1}-\alpha = [J_F(x_k)]^{-1}E_F,$$

so that $\|x_{k+1}-\alpha\|_\infty \leq \mathrm{const.}\|x_k-\alpha\|_\infty^2$, *i.e.* quadratic convergence!

Newton's Method

Example: Newton's method for the two-point Gauss quadrature rule

Recall the system of equations

$$\begin{aligned}
F_1(x_1, x_2, w_1, w_2) &= w_1 + w_2 - 2 = 0 \\
F_2(x_1, x_2, w_1, w_2) &= w_1 x_1 + w_2 x_2 = 0 \\
F_3(x_1, x_2, w_1, w_2) &= w_1 x_1^2 + w_2 x_2^2 - 2/3 = 0 \\
F_4(x_1, x_2, w_1, w_2) &= w_1 x_1^3 + w_2 x_2^3 = 0
\end{aligned}$$

Newton's Method

We can solve this in Matlab using our own implementation of Newton's method

To do this, we require the Jacobian of this system:

$$J_F(x_1, x_2, w_1, w_2) = \begin{bmatrix} 0 & 0 & 1 & 1 \\ w_1 & w_2 & x_1 & x_2 \\ 2w_1x_1 & 2w_2x_2 & x_1^2 & x_2^2 \\ 3w_1x_1^2 & 3w_2x_2^2 & x_1^3 & x_2^3 \end{bmatrix}$$

Newton's Method

Alternatively, we can use Python's built-in `fsolve` function

Note that `fsolve` computes a finite difference approximation to the Jacobian by default

(Or we can pass in an analytical Jacobian if we want)

Matlab has an equivalent `fsolve` function.

Newton's Method

Python example: With either approach and with starting guess $x_0 = [-1, 1, 1, 1]$, we get

```
x_k =
  -0.577350269189626
   0.577350269189626
   1.000000000000000
   1.000000000000000
```

Conditions for Optimality

Existence of Global Minimum

In order to guarantee existence and uniqueness of a global min. we need to make assumptions about the objective function

e.g. if f is continuous on a closed[1] and bounded set $S \subset \mathbb{R}^n$ then it has global minimum in S

In one dimension, this says f achieves a minimum on the interval $[a, b] \subset \mathbb{R}$

In general f does not achieve a minimum on (a, b), *e.g.* consider $f(x) = x$

(Though $\inf_{x \in (a,b)} f(x)$, the largest lower bound of f on (a, b), is well-defined)

[1] A set is closed if it contains its own boundary

Existence of Global Minimum

Another helpful concept for existence of global min. is coercivity

A continuous function f on an unbounded set $S \subset \mathbb{R}^n$ is coercive if

$$\lim_{\|x\| \to \infty} f(x) = +\infty$$

That is, $f(x)$ must be large whenever $\|x\|$ is large

Existence of Global Minimum

If f is coercive on a closed, unbounded[2] set S, then f has a global minimum in S

Proof: From the definition of coercivity, for any $M \in \mathbb{R}$, $\exists r > 0$ such that $f(x) \geq M$ for all $x \in S$ where $\|x\| \geq r$

Suppose that $0 \in S$, and set $M = f(0)$

Let $Y \equiv \{x \in S : \|x\| \geq r\}$, so that $f(x) \geq f(0)$ for all $x \in Y$

And we already know that f achieves a minimum (which is at most $f(0)$) on the closed, bounded set $\{x \in S : \|x\| \leq r\}$

Hence f achieves a minimum on S $\square$

[2] *e.g.* S could be all of $\mathbb{R}^n$, or a "closed strip" in $\mathbb{R}^n$

Existence of Global Minimum

For example:

- $f(x,y) = x^2 + y^2$ is coercive on $\mathbb{R}^2$ (global min. at $(0,0)$)
- $f(x) = x^3$ is not coercive on $\mathbb{R}$ ($f \to -\infty$ for $x \to -\infty$)
- $f(x) = e^x$ is not coercive on $\mathbb{R}$ ($f \to 0$ for $x \to -\infty$)

Question: What about uniqueness?