Applied Mathematics 205

Unit 4. Optimization

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November 2, 2022

Motivation

- This unit will cover nonlinear equations and optimization
- So far we have mostly focused on linear problems
  - linear least squares (linear combination of basis functions)
  - linear physical laws (idealized behavior, small deformations)
  - discretizations of linear PDEs (wave equation, heat equation)
- However, important applications lead to nonlinear problems
  - nonlinear least squares (nonlinear dependency on parameters)
  - nonlinear physical models (realistic materials, large deformations)
  - discretizations of nonlinear PDEs (Navier-Stokes)

Motivation: Nonlinear Equations

- Some familiar problems can be reduced to nonlinear equations
- For example, computing the points and weights of Gauss quadrature

$$\int_{-1}^{1} f(x)\mathrm{d}x \approx \sum_{k=0}^{n} w_k f(x_k)$$

  with $2n+2$ unknown parameters $x_0, \ldots, x_n$ and $w_0, \ldots, w_n$
- Require that quadrature is exact on monomials of degree up to $2n+1$

Motivation: Nonlinear Equations

- For $n = 1$, this leads to a system of nonlinear equations

$$\begin{aligned} w_0 + w_1 &= \int_{-1}^{1} 1\mathrm{d}x = 2 \\ w_0 x_0 + w_1 x_1 &= \int_{-1}^{1} x\mathrm{d}x = 0 \\ w_0 x_0^2 + w_1 x_1^2 &= \int_{-1}^{1} x^2\mathrm{d}x = 2/3 \\ w_0 x_0^3 + w_1 x_1^3 &= \int_{-1}^{1} x^3\mathrm{d}x = 0 \end{aligned}$$

Motivation: Nonlinear Equations

- A general system of m equations for n unknowns

$$F(x) = 0$$

  where $F : \mathbb{R}^n \to \mathbb{R}^m$
- We will focus on the case $m = n$,
  i.e. equal number of equations and unknowns
- Cases $m \neq n$ can be formulated as nonlinear least squares

Motivation: Nonlinear Equations

- One class of nonlinear equations is polynomial equations, i.e. $F(x)$ is a polynomial
- The simplest case is a quadratic equation

$$ax^2 + bx + c = 0$$

- A closed-form solution is given by

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Motivation: Nonlinear Equations

- There are also closed-form solutions for polynomial equations of degree three and four, due to Ferrari and Cardano (~1540)
- However, the Abel–Ruffini theorem states that equations of degree five or higher have no general solution in radicals
- Therefore, they have to be solved numerically with an iterative algorithm

Motivation: Nonlinear Equations

- There are many iterative methods for nonlinear equations
- One is the bisection method for a scalar equation

  $$f(x) = 0$$

  where $f \in C[a, b]$
- Assume $f(a)f(b) < 0$ and bisect the interval depending on the sign of $f(\frac{a+b}{2})$

Motivation: Nonlinear Equations

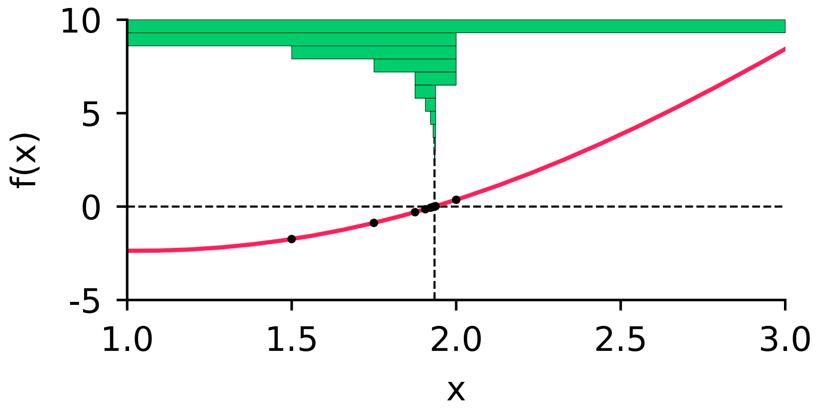
```
def f(x):
    return x * x - 4 * np.sin(x)

# Initial interval, assume f(a)*f(b)<0.
a = 1
b = 3
tol = 1e-3

# Bisection search.
while b - a > tol:
    print('a={:.5f} b={:.5f} f(a)={:.5f} f(b)={:.5f}
          .format(a, b, f(a), f(b)))
    c = 0.5 * (b + a)
    if f(a) * f(c) < 0:
        b = c
    else:
        a = c
```

[examples/unit4/bisection.py]

```
a=1.00000 b=3.00000 f(a)=-2.36588 f(b)=8.43552
a=1.00000 b=2.00000 f(a)=-2.36588 f(b)=0.36281
a=1.50000 b=2.00000 f(a)=-1.73998 f(b)=0.36281
a=1.75000 b=2.00000 f(a)=-0.87344 f(b)=0.36281
a=1.87500 b=2.00000 f(a)=-0.30072 f(b)=0.36281
a=1.87500 b=1.93750 f(a)=-0.30072 f(b)=0.01985
a=1.90625 b=1.93750 f(a)=-0.14326 f(b)=0.01985
a=1.92188 b=1.93750 f(a)=-0.06241 f(b)=0.01985
a=1.92969 b=1.93750 f(a)=-0.02145 f(b)=0.01985
a=1.93359 b=1.93750 f(a)=-0.00085 f(b)=0.01985
a=1.93359 b=1.93555 f(a)=-0.00085 f(b)=0.00949
```



Motivation: Nonlinear Equations

- Bisection is a robust method in 1D,
  but it needs an initial guess $f(a)f(b) < 0$
  and does not generalize to higher dimensions
- We will consider alternative methods
  - fixed-point iteration
  - Newton's method

Motivation: Optimization

- A related topic is optimization
- Has important applications in science and engineering
- Examples
  - find the shape of a racing car that maximizes downforce
  - design a bridge to minimize its weight
  - find the path of an airplane that minimizes fuel consumption
- Solving nonlinear equations can be viewed
  as optimization of the residuals

Motivation: Optimization

- Optimization can be constrained,
  i.e. parameters have to satisfy equations or inequalities
- Examples
  - find the shape of a racing car that maximizes downforce,
    subject to a constant drag
  - design a bridge to minimize its weight,
    subject to a constant critical load
  - find the path of an airplane that minimizes fuel consumption,
    but avoids certain territories

Motivation: Optimization

- All these problems can be formulated as constrained minimization

$$\boxed{\begin{array}{l}\text{Given an objective function } f : \mathbb{R}^n \to \mathbb{R} \text{ and a set } S \subset \mathbb{R}^n, \\ \text{find } x^* \in S \text{ such that } f(x^*) \leq f(x)\ \forall x \in S\end{array}}$$

- Here S is the feasible set which describes the constraints, usually defined by equations or inequalities
- If $S = \mathbb{R}^n$, then the minimization is unconstrained
- Maximization of f is equivalent to minimization of $-f$

Motivation: Optimization

- The standard way to write an optimization problem is

  $$\min_x f(x) \text{ subject to } g(x) = 0 \text{ and } h(x) \le 0$$

  with

  - objective function $f : \mathbb{R}^n \to \mathbb{R}$
  - equality constraints $g : \mathbb{R}^n \to \mathbb{R}^m$
  - inequality constraints $h : \mathbb{R}^n \to \mathbb{R}^p$

Motivation: Optimization

- For example, consider a cylinder with radius x_1 and height x_2
- Minimize the surface area of a cylinder subject to a constraint on its volume

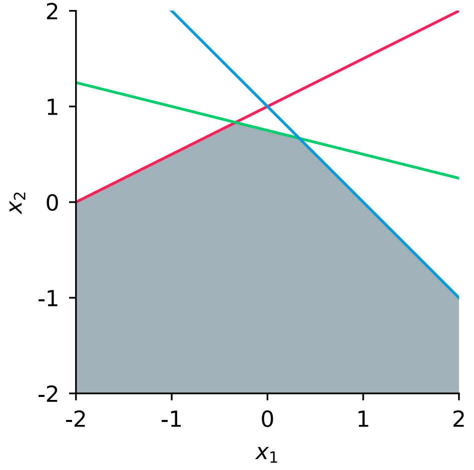
$$\min_{x} f(x_1, x_2) = 2\pi x_1(x_1 + x_2)$$

$$\text{subject to } g(x_1, x_2) = \pi x_1^2 x_2 - V = 0$$

- We will return to this example later

Motivation: Optimization

- If f, g and h are all affine (i.e. $f(x) = Ax + b$, linear plus constant), then the optimization problem is called a linear programming
- Here the term "program" is a synonym for "plan", has nothing to do with computer software
- The feasible set is a polyhedron and the minimum is found on its vertex

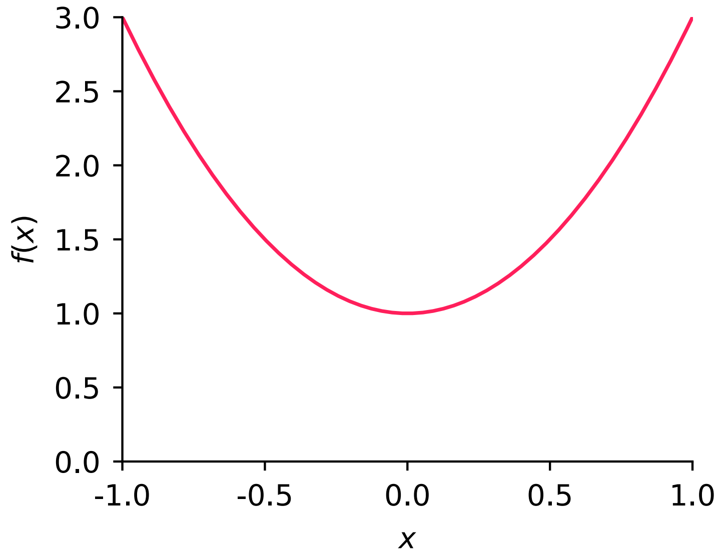


Motivation: Optimization

- If the objective function or any of the constraints are nonlinear
  then we have a nonlinear optimization problem or nonlinear programming
- We will consider several different approaches to nonlinear optimization
- Optimization routines typically use local information
  about a function to iteratively approach its local minimum

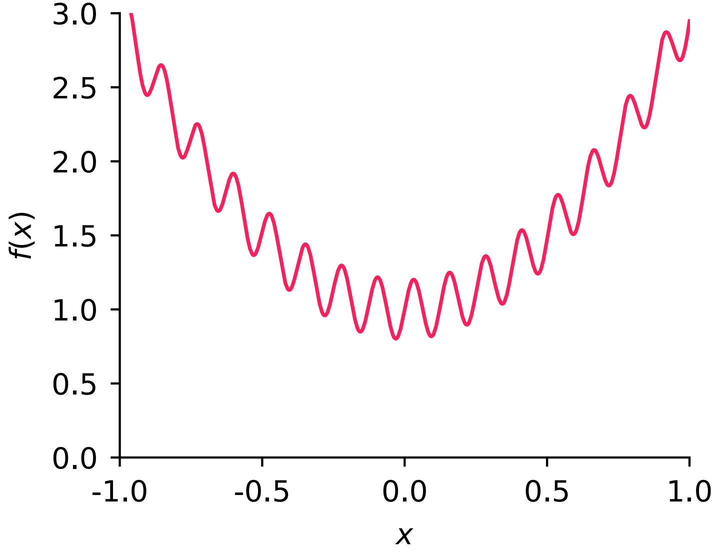
Motivation: Optimization

- In some cases an optimizer can find a global minimum
- Extra conditions on the function (e.g. convexity) can help



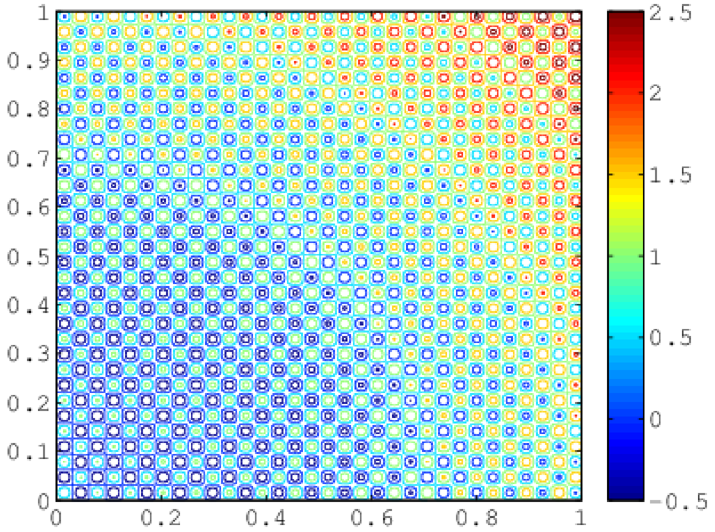
Motivation: Optimization

- But in general, global optimization is difficult
- The optimizer can get “stuck” in local minimum



Motivation: Optimization

- This can get even harder in higher dimensions



Motivation: Optimization

- We will focus on methods for finding local minima
- Global optimization is important, but not possible in general without extra conditions on the objective function
- Global optimization usually relies on heuristics
  - try several different initial guesses (multistart methods)
  - simulated annealing (add decaying noise)
  - genetic methods (use a hierarchy of samples)

Nonlinear Equations

Fixed-Point Iteration

- Consider iteration

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

- For example, recall Heron's method for finding $\sqrt{a}$ from HW0

$$x_{k+1} = \frac{1}{2}\left(x_k + \frac{a}{x_k}\right)$$

- Denote $g_{\text{heron}}(x) = \frac{1}{2}\left(x + a/x\right)$

Fixed-Point Iteration

- Suppose $\alpha \in \mathbb{R}$ is such that $g(\alpha) = \alpha$, then we call α a fixed point of g
- For example, we see that $\sqrt{a}$ is a fixed point of g_{heron} since

$$g_{\text{heron}}(\sqrt{a}) = \frac{1}{2}\left(\sqrt{a} + a/\sqrt{a}\right) = \sqrt{a}$$

- A fixed-point iteration terminates once a fixed point is reached, since if $g(x_k) = x_k$ then we get $x_{k+1} = x_k$
- Also, if $x_{k+1} = g(x_k)$ converges as $k \to \infty$, it must converge to a fixed point
- Let $\alpha = \lim_{k\to\infty} x_k$, then

$$\alpha = \lim_{k\to\infty} x_{k+1} = \lim_{k\to\infty} g(x_k) = g\left(\lim_{k\to\infty} x_k\right) = g(\alpha)$$

Fixed-Point Iteration

- Therefore, for example, if Heron's method converges, it converges to $\sqrt{a}$
- There are sufficient conditions for convergence of a fixed-point iteration
- Recall that g satisfies a Lipschitz condition in an interval $[a, b]$ if

$$|g(x) - g(y)| \leq L|x - y|, \quad \forall x, y \in [a, b]$$

for some $L > 0$

- If $L < 1$, then g is called a contraction

Fixed-Point Iteration

- Theorem: Suppose that g is a contraction on $[\alpha - \delta, \alpha + \delta]$ and α is a fixed point of g (i.e. $g(\alpha) = \alpha$), where $\alpha \in \mathbb{R}$ and $\delta > 0$ Then the fixed point iteration converges to α for any $x_0 \in [\alpha - \delta, \alpha + \delta]$
- Proof: Take $L < 1$ from the Lipschitz condition. Then

$$|x_k - \alpha| = |g(x_{k-1}) - g(\alpha)| \leq L|x_{k-1} - \alpha|,$$

which implies

$$|x_k - \alpha| \leq L^k |x_0 - \alpha|$$

and, since $L < 1$, $|x_k - \alpha| \to 0$ as $k \to \infty$

- This also shows that each iteration reduces the error by factor L

Fixed-Point Iteration

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

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

- We now use this result 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 $|g'|$, for any $\epsilon > 0$, there is $\delta > 0$ such that for any $x \in (\alpha - \delta, \alpha + \delta)$ we have $\big| |g'(x)| - |g'(\alpha)| \big| \leq \epsilon$
- Therefore

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

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

Fixed-Point Iteration

- Furthermore, as $k \to \infty$,

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

- Therefore, asymptotically, after each iteration the error decreases by a factor of $|g'(\alpha)|$

Fixed-Point Iteration

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

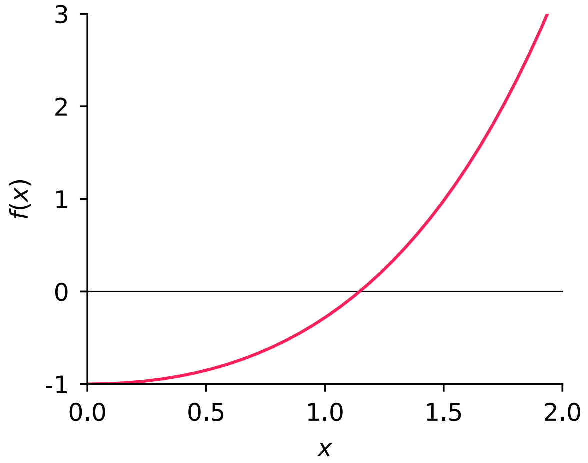
$$\lim_{k\to\infty} \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} = \mu$$

- 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 $f(x) = 0$
- For example, suppose $f(x) = e^x - x - 2$



- From the plot, there is a root at $x \approx 1.15$

Fixed-Point Iteration

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

$$x_{k+1} = \log(x_k + 2)$$

- Here $g(x) = \log(x + 2)$, and $g'(x) = 1/(x + 2) < 1$ for all $x > -1$, therefore fixed point iteration will converge for $x_0 > -1$
- We should get linear convergence with a factor about

$$g'(1.15) = 1/(1.15 + 2) \approx 0.32$$

Fixed-Point Iteration

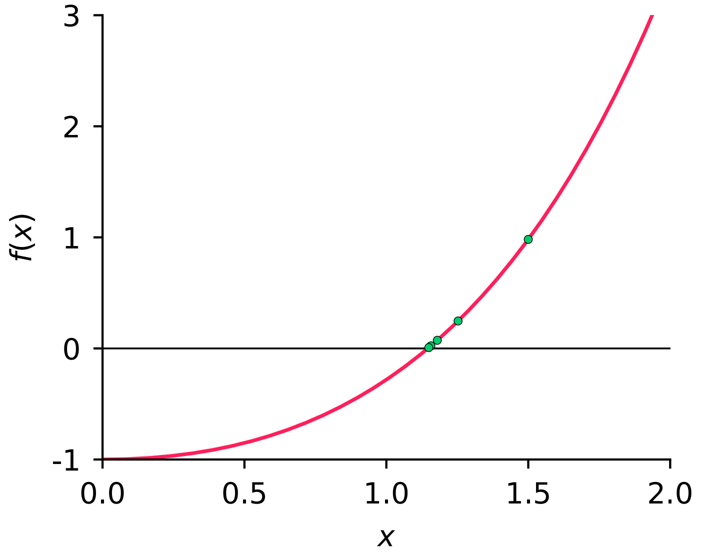
- An alternative fixed-point iteration is to set

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

- Therefore $g(x) = e^x - 2$, and $g'(x) = e^x$
- Hence $|g'(\alpha)| > 1$, so we can't guarantee convergence
- In fact, the iteration diverges

Fixed-Point Iteration

- See [examples/unit4/fixed_point.py], comparison of the two fixed-point iterations



Newton's Method

- Constructing fixed-point iterations is not straightforward
- Need to rewrite $f(x) = 0$ in a form $x = g(x)$ with certain properties on g
- To obtain a more generally applicable iterative method, consider the following fixed-point iteration

$$x_{k+1} = x_k - \lambda(x_k) f(x_k)$$

  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 want

Newton's Method

- Recall that the asymptotic convergence rate is dictated by $|g'(\alpha)|$, so we want to have $|g'(\alpha)| = 0$ to get superlinear convergence
- Suppose (as stated above) that $f(\alpha) = 0$, then

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

- To satisfy $g'(\alpha) = 0$, we choose $\lambda(x) = 1/f'(x)$ to obtain

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

known as Newton's method

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 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

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

- Therefore, asymptotically,
  the error at iteration $k+1$ is the square of the error at iteration k
- This is referred to as quadratic convergence, which is very rapid
- We need to be sufficiently close to α to get quadratic convergence (the 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 the secant methods are
  - does not require computing $f'(x)$
  - requires only one extra evaluation of $f(x)$ per solution (Newton's method also requires $f'(x_k)$ each iteration)

Secant Method

- As one may expect, the secant method 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 $q \approx 1.6$
- See [examples/unit4/secant_vs_newton.py],
  Newton's method versus secant method for $f(x) = e^x - x - 2$

Systems of Nonlinear Equations

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 $\alpha \in \mathbb{R}^n$ such that $F(\alpha) = 0$
- In component form, this is equivalent to

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

Fixed-Point Iteration

- For a fixed-point iteration, we again 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 $\|x_k - \alpha\| \leq L^k\|x_0 - \alpha\|$
- 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: Example

- Once again, we can employ a fixed point iteration to solve $F(x) = 0$
- For example, 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: Example

- Define

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

- See [examples/unit4/fixed_point_2d.py], fixed-point iteration in two dimensions

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

$$x_{k+1} = x_k - J_F(x_k)^{-1} F(x_k)$$

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

$$J_F(x_k)\Delta x_{k+1} = -F(x_k)$$

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

Newton's Method

- Once again, if x_0 is sufficiently close to α, then Newton's method converges quadratically
- This result again relies on Taylor's theorem
- We first consider how to generalize Taylor's theorem to $\mathbb{R}^n$
- First, we consider the case for $F : \mathbb{R}^n \to \mathbb{R}$

Multivariate Taylor Theorem

- Let $\phi(s) = F(x + s\delta)$ and $\delta \in \mathbb{R}^n$. One-dimensional Taylor theorem yields

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

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

Multivariate Taylor Theorem

- We have

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

where

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

and

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

Multivariate Taylor Theorem

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

$$\begin{aligned}
|E_k| &\le \frac{1}{(k+1)!}\left|\left[\left(\|\delta\|_\infty \frac{\partial}{\partial x_1} + \ldots + \|\delta\|_\infty \frac{\partial}{\partial x_n}\right)^{k+1} F\right](x+\eta\delta)\right| \\
&= \frac{1}{(k+1)!}\|\delta\|_\infty^{k+1}\left|\left[\left(\frac{\partial}{\partial x_1} + \ldots + \frac{\partial}{\partial x_n}\right)^{k+1} F\right](x+\eta\delta)\right| \\
&\le \frac{n^{k+1}}{(k+1)!} A\|\delta\|_\infty^{k+1}
\end{aligned}$$

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

Multivariate Taylor Theorem

- We 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 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

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

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 $\|E_F\|_\infty = \max\limits_{1 \le i \le n} |E_{i,1}| \le \frac{1}{2} n^2 \left(\max\limits_{1 \le i,j,\ell \le n} \left| \frac{\partial^2 F_i}{\partial x_j \partial x_\ell} \right| \right) \|\delta\|_\infty^2$

Newton's Method

- Now return to Newton's method
- We have

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

  so that

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

Newton's Method

- Also, the Newton iteration itself can be rewritten as

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

- We obtain

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

which implies quadratic convergence

$$\|x_{k+1}-\alpha\|_\infty \leq C\|x_k-\alpha\|_\infty^2$$

Newton's Method: Example

- Recall the conditions of the two-point Gauss quadrature rule

$$\begin{aligned}F_1(x_1,x_2,w_1,w_2) &= w_1 + w_2 - 2 = 0\\ F_2(x_1,x_2,w_1,w_2) &= w_1x_1 + w_2x_2 = 0\\ F_3(x_1,x_2,w_1,w_2) &= w_1x_1^2 + w_2x_2^2 - 2/3 = 0\\ F_4(x_1,x_2,w_1,w_2) &= w_1x_1^3 + w_2x_2^3 = 0\end{aligned}$$

- They constitute a nonlinear system of 4 equations for 4 unknowns

Newton's Method: Example

- We can solve this using Newton's method
- To do this, we require the Jacobian of this system:

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

- Alternatively, use `scipy.optimize.fsolve()` that implements Powell's hybrid method (combination of Newton and gradient descent) by calling HYBRD or HYBRJ from Fortran library MINPACK
- See [examples/unit4/nonlin_gauss_quad.py], two-point Gauss quadrature found from a nonlinear system

Newton's Method: Example

- Using either approach with an initial guess $[-1, 1, 1, 1]$, we get the solution

$$\begin{aligned} x_1 &= -0.577350269189626 &\approx -1/\sqrt{3} \\ x_2 &= 0.577350269189626 &\approx 1/\sqrt{3} \\ w_1 &= 1.000000000000000 &\approx 1 \\ w_2 &= 1.000000000000000 &\approx 1 \end{aligned}$$

Optimization

Existence of Global Minimum

- To guarantee existence and uniqueness of a global minimum, we need to make assumptions about the objective function
- For example, if f is continuous on a closed (i.e. $\partial S \subset S$) 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 $f(x) = x$

Coercive Functions

- Another helpful concept for existence of global minimum is coercivity
- A function $f : S \to \mathbb{R}$ on an unbounded set $S \subset \mathbb{R}^n$ is coercive if

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

- That is, $f(x)$ must take large positive values whenever $\|x\|$ is large

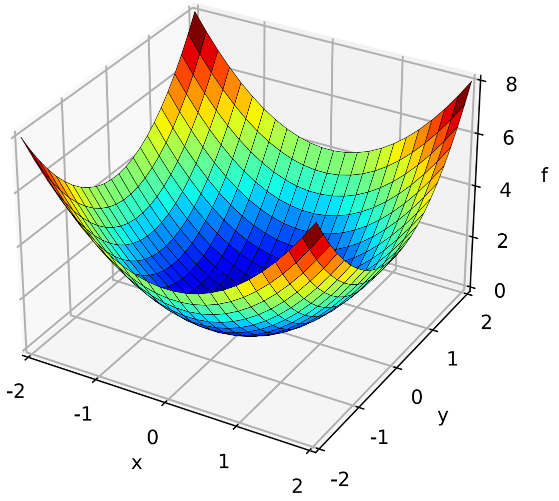
Coercive Functions

- If f is continuous and coercive on a closed 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 $\|x\| \geq r$
- Take a point $x_0 \in S$, and set $M = f(x_0)$
- Let $Y = S \cap \{\|x\| \geq r\}$, so that $f(x) \geq f(x_0)$ for all $x \in Y$
- And we already know that f achieves a minimum (which is at most $f(x_0)$) on the closed and bounded set $S \cap \{\|x\| \leq r\}$
- Hence f achieves a minimum on S $\square$

Coercive Functions: Examples

$f = x^2 + y^2$

coercive on $\mathbb{R}^2$

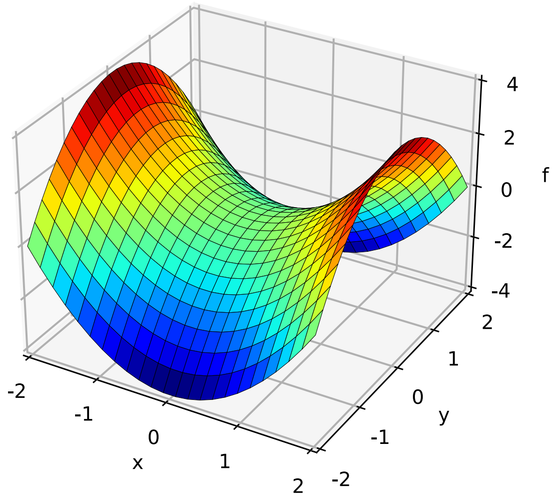


$f = x^2 - y^2$

not coercive on $\mathbb{R}^2$

$f(0, y) \to -\infty$

as $|y| \to \infty$

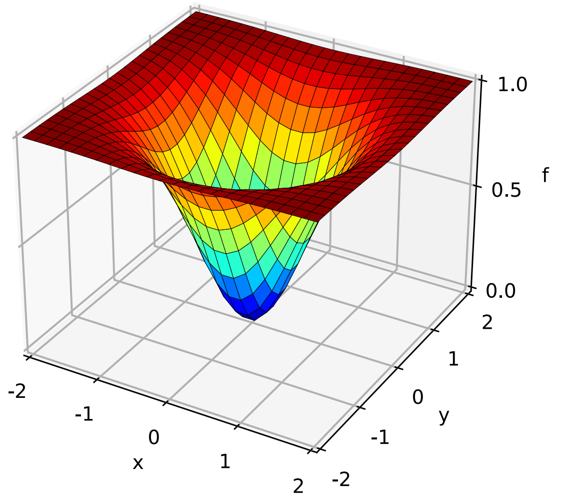


$f = 1 - e^{-(x^2+y^2)}$

not coercive on $\mathbb{R}^2$

$f(x, y) \to 1$

as $x^2 + y^2 \to \infty$



Convex Functions

- An important concept for uniqueness is convexity
- A set $S \subset \mathbb{R}^n$ is convex if it contains the line segment between any two of its points
- That is, S is convex if for any $x, y \in S$, we have

$$\{\theta x + (1-\theta)y : \theta \in [0,1]\} \subset S$$

Convex Functions

- Similarly, we define convexity of a function $f : S \subset \mathbb{R}^n \to \mathbb{R}$
- f is convex if its graph along any line segment in S is on or below the chord connecting the function values
- For example, f is convex if for any $x, y \in S$ and any $\theta \in (0, 1)$, we have

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y)$$

- Also, if

$$f(\theta x + (1-\theta)y) < \theta f(x) + (1-\theta) f(y)$$

  then f is strictly convex

Convex Functions: Examples

$f = x^2 + y^2$

convex on $\mathbb{R}^2$

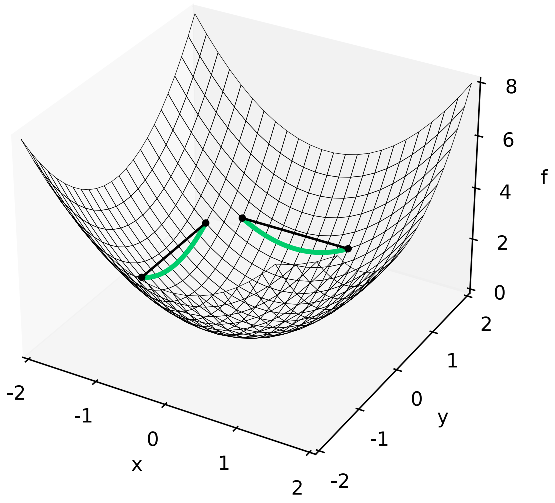
$f = x^2 - y^2$

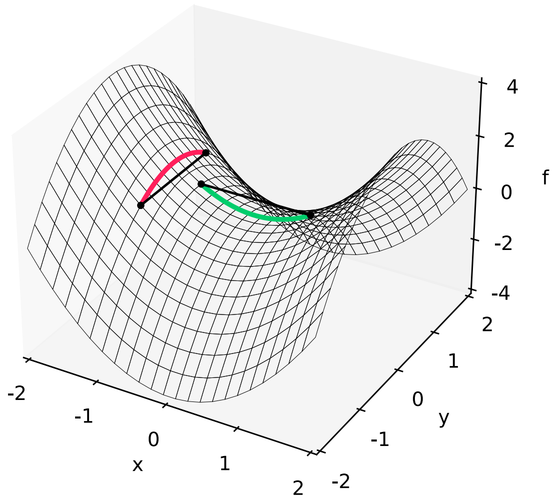
not convex on $\mathbb{R}^2$

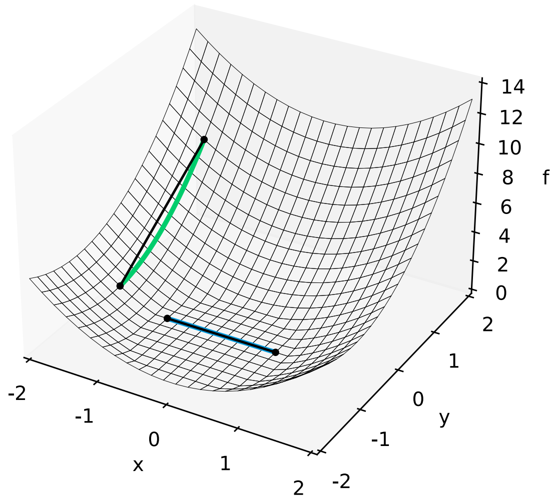
$f = \max(1,\ x^2 + (y+1)^2)$

convex but

not strictly convex on $\mathbb{R}^2$







Convex Functions

- If f is a convex function on a convex set S, then any local minimum of f must be a global minimum
- Proof (1/2): Suppose x is a local minimum, i.e. there is $\epsilon > 0$ so that $f(x) \leq f(y)$ for $y \in B(x, \epsilon)$, where $B(x, \epsilon) = \{y \in S : \|y - x\| \leq \epsilon\}$
- Suppose that x is not a global minimum, i.e. that there exists $w \in S$ such that $f(w) < f(x)$
- We will show that this gives a contradiction by drawing a line segment between x and w

Convex Functions

Proof (2/2):

- For $\theta \in [0,1]$ we have $f(\theta w + (1-\theta)x) \leq \theta f(w) + (1-\theta) f(x)$
- Let $\sigma \in (0,1]$ be sufficiently small so that

$$z = \sigma w + (1-\sigma)\, x \in B(x, \epsilon)$$

- Then

$$f(z) \leq \sigma f(w) + (1-\sigma)\, f(x) < \sigma f(x) + (1-\sigma)\, f(x) = f(x),$$

  e.g. $f(z) < f(x)$, which contradicts that $f(x)$ is a local minimum
- Hence we cannot have $w \in S$ such that $f(w) < f(x)$ $\square$

Convex Functions

- Note that convexity does not guarantee uniqueness of global minimum
- However, if f is a strictly convex function on a convex set S, then a local minimum of f is the unique global minimum
- Optimization of convex functions over convex sets is called convex optimization, which is an important field in optimization

Optimality Conditions

- We have discussed existence and uniqueness of minima,
  but haven't considered how to find a minimum
- The familiar optimization idea from calculus in one dimension is:
  set derivative to zero, check the sign of the second derivative
- This can be generalized to $\mathbb{R}^n$

Optimality Conditions

- If $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable, then the gradient vector $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$ is

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

- The importance of the gradient is that ∇f points "uphill", i.e. towards points with larger values than $f(x)$
- And similarly $-\nabla f$ points "downhill"

Optimality Conditions

- This follows from Taylor's theorem for $f : \mathbb{R}^n \to \mathbb{R}$
- Recall that

$$f(x+\delta) - f(x) = \nabla f(x)^T \delta + \text{h.o.t.}$$

- Let $\delta = -\epsilon \nabla f(x)$ for $\epsilon > 0$ and suppose that $\nabla f(x) \neq 0$, then:

$$f(x - \epsilon \nabla f(x)) - f(x) \approx -\epsilon \nabla f(x)^T \nabla f(x) < 0$$

- Also, we see from Cauchy–Schwarz that

$$\left| \nabla f(x)^T \frac{\delta}{\|\delta\|_2} \right| \leq \left| \nabla f(x)^T \frac{\nabla f(x)}{\|\nabla f(x)\|_2} \right|$$

so $-\nabla f(x)$ is the steepest descent direction

Optimality Conditions

- Similarly, we see that a necessary condition for a local minimum at $x^* \in S$ is that $\nabla f(x^*) = 0$
- In this case there is no “downhill direction” at x^*
- The condition $\nabla f(x^*) = 0$ is called a first-order necessary condition for optimality, since it only involves first derivatives

Optimality Conditions

- $x^* \in S$ that satisfies the first-order optimality condition is called a critical point of f
- A critical point can be a local minimum, local maximum, or saddle point
- A saddle point is where some directions are "downhill" and others are "uphill", e.g. $(x, y) = (0, 0)$ for $f(x, y) = x^2 - y^2$

Optimality Conditions

- As in the one-dimensional case, we can look at second derivatives to classify critical points
- If $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable, then the Hessian is the matrix-valued function $H_f : \mathbb{R}^n \to \mathbb{R}^{n \times n}$

$$H_f(x) = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n x_1} & \frac{\partial^2 f(x)}{\partial x_n x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

- The Hessian is the Jacobian matrix of the gradient $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$
- If the second partial derivatives of f are continuous, then $\partial^2 f / \partial x_i \partial x_j = \partial^2 f / \partial x_j \partial x_i$, and H_f is symmetric

Optimality Conditions

- Suppose we have found a critical point x^*, so that $\nabla f(x^*) = 0$
- From Taylor's theorem, for $\delta \in \mathbb{R}^n$, we have

$$\begin{aligned} f(x^* + \delta) &= f(x^*) + \nabla f(x^*)^T \delta + \frac{1}{2}\delta^T H_f(x^* + \eta\delta)\delta \\ &= f(x^*) + \frac{1}{2}\delta^T H_f(x^* + \eta\delta)\delta \end{aligned}$$

for some $\eta \in (0, 1)$

Optimality Conditions

- Recall positive definiteness: A is positive definite if $x^T Ax > 0$
- Suppose $H_f(x^*)$ is positive definite
- Then (by continuity) $H_f(x^* + \eta\delta)$ is also positive definite for $\|\delta\|$ sufficiently small, so that: $\delta^T H_f(x^* + \eta\delta)\delta > 0$
- Hence, we have $f(x^* + \delta) > f(x^*)$ for $\|\delta\|$ sufficiently small, e.g. $f(x^*)$ is a local minimum
- Positive definiteness of H_f at a critical point x^* is a second-order sufficient condition for a local minimum

Optimality Conditions

- A matrix can also be negative definite: $x^T Ax < 0$ for all $x \neq 0$
- Or indefinite: There exists x, y such that $x^T Ax < 0 < y^T Ay$
- Then we can classify critical points as follows:
  - $H_f(x^*)$ positive definite $\implies$ x^* is a local minimum
  - $H_f(x^*)$ negative definite $\implies$ x^* is a local maximum
  - $H_f(x^*)$ indefinite $\implies$ x^* is a saddle point

Optimality Conditions

- Also, positive definiteness of the Hessian is closely related to convexity of f
- If $H_f(x)$ is positive definite, then f is convex on some convex neighborhood of x
- If $H_f(x)$ is positive definite for all $x \in S$, where S is a convex set, then f is convex on S
- Question: How do we test for positive definiteness?

Optimality Conditions

- Answer: For a symmetric matrix A
  - A is positive definite if and only if all eigenvalues of A are positive,
  - A is negative definite if and only if all eigenvalues of A are negative
- Also, a matrix with positive and negative eigenvalues is indefinite
- Hence we can compute all the eigenvalues of A and check their signs

Optimality Conditions: Example

- From Heath's book (Example 6.5)
- Consider

$$f(x) = 2x_1^3 + 3x_1^2 + 12x_1x_2 + 3x_2^2 - 6x_2 + 6$$

- Then

$$\nabla f(x) = \begin{bmatrix} 6x_1^2 + 6x_1 + 12x_2 \\ 12x_1 + 6x_2 - 6 \end{bmatrix}$$

- We set $\nabla f(x) = 0$ to find critical points $[1, -1]^T$ and $[2, -3]^T$

Optimality Conditions: Example

- The Hessian is

$$H_f(x) = \begin{bmatrix} 12x_1 + 6 & 12 \\ 12 & 6 \end{bmatrix}$$

- and hence

$$H_f(1,-1) = \begin{bmatrix} 18 & 12 \\ 12 & 6 \end{bmatrix}, \text{ which has eigenvalues } 25.4, -1.4$$

$$H_f(2,-3) = \begin{bmatrix} 30 & 12 \\ 12 & 6 \end{bmatrix}, \text{ which has eigenvalues } 35.0, 1.0$$

- Hence $[2,-3]^T$ is a local minimum whereas $[1,-1]^T$ is a saddle point

Optimization Methods

Steepest Descent

- One gradient-based method for unconstrained optimization is steepest descent
- Key idea: The negative gradient $-\nabla f(x)$ points in the "steepest downhill" direction for f at x
- An iterative method for minimizing f is obtained by following $-\nabla f(x_k)$ at each step
- Question: How far should we go in the direction of $-\nabla f(x_k)$?

Steepest Descent

- We can try to find the best step size via an easier subproblem
- For a direction $s \in \mathbb{R}^n$, let $\phi : \mathbb{R} \to \mathbb{R}$ be given by

$$\phi(\eta) = f(x + \eta s)$$

- Then minimizing f along s corresponds
  to minimizing the one-dimensional function ϕ
- This process of minimizing f along a line is called a line search

Steepest Descent

- Putting these pieces together leads to the steepest descent method:

```
1: choose initial guess $x_0$
2: **for** $k = 0, 1, 2, \ldots$ **do**
3:     $s_k = -\nabla f(x_k)$
4:     choose $\eta_k$ to minimize $f(x_k + \eta_k s_k)$
5:     $x_{k+1} = x_k + \eta_k s_k$
6: **end for**
```

- However, steepest descent often converges very slowly
- Steepest descent is part of HW4
- A simpler option to use a constant $\eta_k = \eta$

Newton's Method

- We can get faster convergence by using more information about f
- Note that $\nabla f(x) = 0$ is a system of nonlinear equations, so we can solve it with quadratic convergence via Newton's method
- The Jacobian matrix of $\nabla f(x)$ is $H_f(x)$ and therefore Newton's method for unconstrained optimization is:

```
1: choose initial guess $x_0$
2: **for** $k = 0, 1, 2, \ldots$ **do**
3:     solve $H_f(x_k)s_k = -\nabla f(x_k)$
4:     $x_{k+1} = x_k + s_k$
5: **end for**
```

Newton's Method

- We can also interpret Newton's method as seeking a stationary point based on a sequence of local quadratic approximations
- Recall that for small δ

$$f(x+\delta) \approx f(x) + \nabla f(x)^T \delta + \frac{1}{2}\delta^T H_f(x)\delta = q(\delta)$$

  where $q(\delta)$ is quadratic in δ (for a fixed x)
- We find stationary point of q in the usual way:

$$\nabla q(\delta) = \nabla f(x) + H_f(x)\delta = 0$$

- This leads to $H_f(x)\delta = -\nabla f(x)$, as in the previous slide

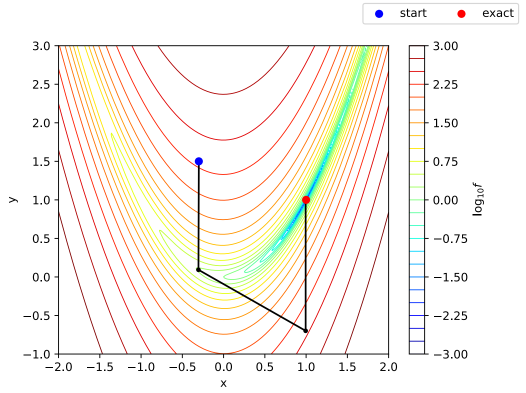
Newton's Method: Example

- Rosenbrock function

$$f(x, y) = 100(y - x^2)^2 + (1 - x)^2$$

with minimum 0 at $(x, y) = (1, 1)$

- See [examples/unit4/rosenbrock.py],
Rosenbrock function minimized with Newton's method



Newton’s Method: Robustness

- Newton’s method generally converges much faster than steepest descent
- However, Newton’s method can be unreliable far away from a solution
- To improve robustness during early iterations
  it is common to perform a line search in the Newton step direction
- Also line search can ensure we don’t approach a local maximum
  (instead of minimum) as can happen with raw Newton method
- The line search modifies the Newton step size,
  therefore often referred to as a damped Newton method

Newton's Method: Robustness

- Another way to improve robustness is with trust region methods
- At each iteration k, a "trust radius" R_k is computed
- This determines a region surrounding x_k
  on which we "trust" our quadratic approx.
- We require $\|x_{k+1} - x_k\| \leq R_k$,
  which is a constrained optimization problem
  (with quadratic objective function) at each step

Newton's Method: Robustness

- Size of R_{k+1} is based on comparing actual change, $f(x_{k+1}) - f(x_k)$, to change predicted by the quadratic model
- If quadratic model is accurate, we expand the trust radius, otherwise we contract it
- When close to a minimum, R_k should be large enough to allow full Newton steps $\implies$ eventual quadratic convergence

Quasi-Newton Methods

- Possible drawbacks of Newton's method
  - unreliable: only converges when sufficiently close to a minimum
  - expensive: the Hessian H_f is dense in general, making the method expensive if n is large
  - complicated: can be impractical to compute the Hessian exactly
- Methods that do not require the Hessian but achieve superlinear convergence are quasi-Newton methods

Quasi-Newton Methods

- General form of quasi-Newton methods:

$$x_{k+1} = x_k - \alpha_k B_k^{-1} \nabla f(x_k)$$

  where α_k is a line search parameter and
  B_k is some approximation to the Hessian
- Quasi-Newton methods generally lose quadratic convergence of Newton's method, but often achieve superlinear convergence
- We now consider some specific quasi-Newton methods

BFGS

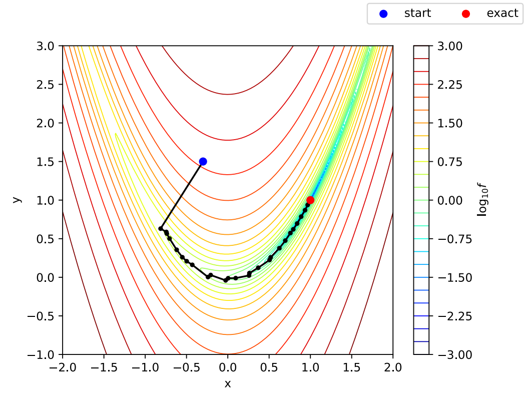
- The Broyden–Fletcher–Goldfarb–Shanno (BFGS) method is one of the most popular quasi-Newton methods

```
1: choose initial guess $x_0$
2: choose $B_0$, initial guess for Hessian, e.g. $B_0 = \mathrm{I}$
3: **for** $k = 0, 1, 2, \ldots$ **do**
4:     solve $B_k s_k = -\nabla f(x_k)$
5:     $x_{k+1} = x_k + s_k$
6:     $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$
7:     $B_{k+1} = B_k + \Delta B_k$
8: **end for**
```

where $\Delta B_k = \frac{y_k y_k^T}{y_k^T s_k} - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k}$

BFGS

- Basic idea is that B_k accumulates second derivative information on successive iterations and eventually approximates H_f well
- BFGS is implemented in `scipy.optimize.fmin_bfgs()`
- See [examples/unit4/rosenbrock.py], Rosenbrock function minimized with BFGS



BFGS: Derivation

- Replace Newton's update $H_f(x_k)s_k = -\nabla f(x_k)$ with

$$B_k s_k = -\nabla f(x_k)$$

  where $s_k = x_{k+1} - x_k$

- Define $B_{k+1} \in \mathbb{R}^{n\times n}$ to satisfy the requirements
  - B_{k+1} is obtained by a "small" change from B_k
  - B_{k+1} is symmetric and positive definite
  - $B_{k+1} \approx H_f(x_{k+1})$

BFGS: Derivation

- In particular, we want $B_{k+1}s_k \approx H_f(x_{k+1})s_k$
- The product $H_f(x_{k+1})s_k$ is the directional derivative of ∇f along s_k and can be approximated by the difference $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$

$$H_f(x_{k+1})s_k = \lim_{h\to 0} \frac{\nabla f(x_{k+1}) - \nabla f(x_{k+1} - hs_k)}{h} \underset{h=1}{\approx} \nabla f(x_{k+1}) - \nabla f(x_k) = y_k$$

- Impose the requirement $B_{k+1}s_k = y_k$ exactly

BFGS: Derivation

- Look for B_{k+1} in the form of a rank-two update

$$B_{k+1} = B_k - \beta v v^T + \alpha u u^T$$

  with unknown $\alpha, \beta \in \mathbb{R}$ and $u, v \in \mathbb{R}^n$
  - impose $(B_k - \beta v v^T) s_k = 0$

    $$0 = (B_k - \beta v v^T) s_k = B_k s_k - \beta v v^T s_k = B_k s_k - (\beta v^T s_k) v$$

    which is achieved by $v = B_k s_k$ and $\beta = \frac{1}{s_k^T B_k s_k}$
  - impose $\alpha u u^T s_k = y_k$

    $$y_k = \alpha u u^T s_k = (\alpha u^T s_k) u$$

    which is achieved by $u = y_k$ and $\alpha = \frac{1}{y_k^T s_k}$
- This implies $B_{k+1} s_k = y_k$ and recovers the BFGS algorithm above

BFGS: Derivation

- Note that if B_k is symmetric and positive definite, then $B_k - \beta vv^T = B_k - \frac{B_k s_k^T s_k^T B_k}{s_k^T B_k s_k}$ is positive semi-definite
- Under the assumption $y_k^T s_k > 0$, known as the curvature condition, the matrix $\alpha uu^T = \frac{y_k y_k^T}{y_k^T s_k}$ is positive definite
- Therefore, $B_{k+1} = B_k - \beta vv^T + \alpha uu^T$ is positive definite

BFGS: Inverse Hessian

- Actual implementation of BFGS: store and update the inverse approximate Hessian H_k to avoid solving a linear system

```
1: choose initial guess $x_0$
2: choose $H_0$, initial guess for inverse Hessian, e.g. $H_0 = \mathrm{I}$
3: **for** $k = 0, 1, 2, \ldots$ **do**
4:     $s_k = -H_k \nabla f(x_k)$
5:     $x_{k+1} = x_k + s_k$
6:     $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$
7:     $H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T$
8: **end for**
```

where $\rho_k = \frac{1}{y_k^T s_k}$

BFGS: Inverse Hessian

- The update rule for H_{k+1} follows from the update rule for B_{k+1} and the Sherman–Morrison–Woodbury formula

$$(A + UV^T)^{-1} = A^{-1} - A^{-1}U(I + V^T A^{-1}U)^{-1}V^T A^{-1}$$

where $A \in \mathbb{R}^{n\times n}$ and $U, V \in \mathbb{U}^{n\times p}$

- Provides a low-rank update of the inverse from a low-rank update of the matrix
- In our case

$$B_{k+1} = B_k + UV^T = B_k + \frac{1}{y_k^T s_k} y_k y_k^T - \frac{1}{s_k^T B_k s_k} B_k s_k s_k^T B_k$$

$$U = \left[\frac{1}{y_k^T s_k} y_k \quad -\frac{1}{s_k^T B_k s_k} B_s s_k\right], \quad V = \begin{bmatrix} y_k & B_k s_k \end{bmatrix} \in \mathbb{R}^{n\times 2}$$

BFGS: Modifications

- Typically, the search direction s_k is adjusted by a more robust inexact line search, e.g. Wolfe conditions
- Limited-memory BFGS (L-BFGS) avoids storing the full H_k and instead represents H_k implicitly using a limited history of gradient evaluations. Suited for large-scale problems
- Extra reading: Nocedal & Wright. *Numerical Optimization*, 1999 (chapters 6 and 7)

Constrained Optimization

Constrained Optimization

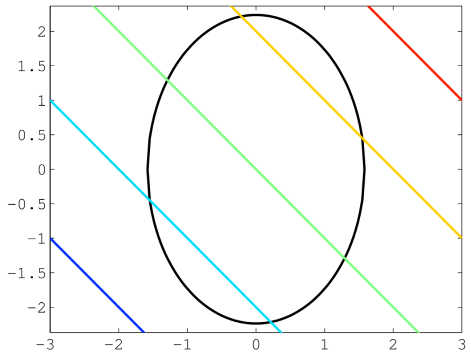
- So far we have ignored constraints
- Now we consider equality constrained optimization

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad g(x) = 0,$$

  where $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$, with $m \leq n$
- There are n unknowns and m constraints
- This problem is solved with Lagrange mutlipliers

Constrained Optimization

- We illustrate the concept of Lagrange multipliers for $f, g : \mathbb{R}^2 \to \mathbb{R}$
- Let $f(x, y) = x + y$ and $g(x, y) = 2x^2 + y^2 - 5$



- ∇g is normal to S: at any $x \in S$ we must move in direction $(\nabla g(x))_\perp$ (tangent direction) to remain in S

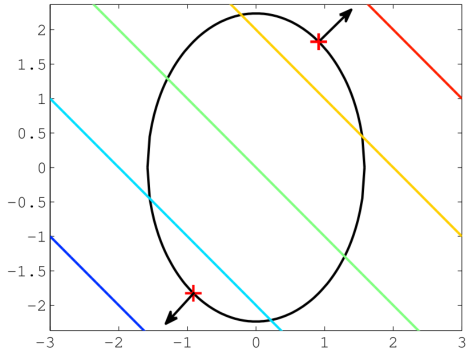
Constrained Optimization

- Also, change in f due to infinitesimal step in direction $(\nabla g(x))_\perp$ is

$$f(x \pm \epsilon(\nabla g(x))_\perp) = f(x) \pm \epsilon \nabla f(x)^T (\nabla g(x))_\perp + \text{h.o.t.}$$

- A critical point $x^* \in S$ satisfies $\nabla f(x^*)^T (\nabla g(x^*))_\perp = 0$, or

$$\nabla f(x^*) = \lambda^* \nabla g(x^*), \quad \text{for some } \lambda^* \in \mathbb{R}$$



Constrained Optimization

- This shows that for a stationary point with $m = 1$ constraints, ∇f cannot have any component in the "tangent direction" to S
- Now, consider the case with $m > 1$ equality constraints
- Then $g : \mathbb{R}^n \to \mathbb{R}^m$ and we have the gradients ∇g_i, $i = 1, \ldots, m$
- Then the feasible set is $S = \{x \in \mathbb{R}^n : g_i(x) = 0, i = 1, \ldots, m\}$
- Any "tangent direction" at $x \in S$ must be orthogonal to all gradient vectors $\{\nabla g_i(x), i = 1, \ldots, m\}$ to remain in S

Constrained Optimization

- Let $\mathcal{T}(x) = \{v \in \mathbb{R}^n : \nabla g_i(x)^T v = 0, i = 1, 2, \ldots, m\}$ denote the orthogonal complement of $\{\nabla g_i(x), i = 1, \ldots, m\}$
- Then, for $\delta \in \mathcal{T}(x)$ and $\epsilon > 0$, $\epsilon\delta$ is a step in a "tangent direction" of S at x
- Since we have

$$f(x^* + \epsilon\delta) = f(x^*) + \epsilon \nabla f(x^*)^T \delta + \text{h.o.t.}$$

it follows that for a stationary point we need

$$\nabla f(x^*)^T \delta = 0 \text{ for all } \delta \in \mathcal{T}(x^*)$$

Constrained Optimization

- We require that at a stationary point $x^* \in S$ we have

$$\nabla f(x^*) \in \operatorname{span}\{\nabla g_i(x^*), i = 1, \ldots, m\}$$

- This can be written as a linear system

$$\nabla f(x^*) = (J_g(x^*))^T \lambda^*$$

  for some $\lambda^* \in \mathbb{R}^m$, where $(J_g(x^*))^T \in \mathbb{R}^{n\times m}$

- This follows because the columns of $(J_g(x^*))^T$ are the vectors $\{\nabla g_i(x^*), i = 1, \ldots, m\}$

Constrained Optimization

- We can write equality constrained optimization problems more concisely by introducing the Lagrangian function, $\mathcal{L} : \mathbb{R}^{n+m} \to \mathbb{R}$,

$$\begin{aligned} \mathcal{L}(x, \lambda) &= f(x) + \lambda^T g(x) \\ &= f(x) + \lambda_1 g_1(x) + \cdots + \lambda_m g_m(x) \end{aligned}$$

- Then

$$\begin{aligned} \frac{\partial \mathcal{L}(x,\lambda)}{\partial x_i} &= \frac{\partial f(x)}{\partial x_i} + \lambda_1 \frac{\partial g_1(x)}{\partial x_i} + \cdots + \lambda_n \frac{\partial g_n(x)}{\partial x_i}, & i = 1, \ldots, n \\ \frac{\partial \mathcal{L}(x,\lambda)}{\partial \lambda_i} &= g_i(x), & i = 1, \ldots, m \end{aligned}$$

Constrained Optimization

- In matrix form

$$\nabla \mathcal{L}(x,\lambda) = \begin{bmatrix} \nabla_x \mathcal{L}(x,\lambda) \\ \nabla_\lambda \mathcal{L}(x,\lambda) \end{bmatrix} = \begin{bmatrix} \nabla f(x) + J_g(x)^T \lambda \\ g(x) \end{bmatrix},$$

- Therefore, the first order necessary optimality condition for the constrained problem can be written as a nonlinear system

$$\nabla \mathcal{L}(x,\lambda) = \begin{bmatrix} \nabla f(x) + J_g(x)^T \lambda \\ g(x) \end{bmatrix} = 0$$

Constrained Optimization: Examples

- Consider a cylinder with radius x_1 and height x_2
- Minimize the surface area of a cylinder subject to a constraint on its volume

$$\min_{x} f(x_1, x_2) = 2\pi x_1 (x_1 + x_2)$$

$$\text{subject to } g(x_1, x_2) = \pi x_1^2 x_2 - V = 0$$

Constrained Optimization: Examples

- Another example is the underdetermined linear least squares problem from Unit 1

$$\min_{b \in \mathbb{R}^n} f(b) \quad \text{subject to} \quad g(b) = 0,$$

where $f(b) = b^T b$, $g(b) = Ab - y$ and $A \in \mathbb{R}^{m \times n}$ with $m < n$

Constrained Optimization: Examples

- Introducing Lagrange multipliers gives

$$\mathcal{L}(b,\lambda) = b^T b + \lambda^T (Ab - y)$$

  where $b \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}^m$

- And the necessary optimality condition $\nabla \mathcal{L}(b,\lambda) = 0$ is

$$\begin{bmatrix} \nabla f(b) + J_g(b)^T \lambda \\ g(b) \end{bmatrix} = \begin{bmatrix} 2b + A^T \lambda \\ Ab - y \end{bmatrix} = 0 \in \mathbb{R}^{n+m}$$

Constrained Optimization: Examples

- We obtain the $(n+m) \times (n+m)$ square linear system

$$\begin{bmatrix} 2\mathrm{I} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ y \end{bmatrix}$$

  which we can solve for $\begin{bmatrix} b \\ \lambda \end{bmatrix} \in \mathbb{R}^{n+m}$

Constrained Optimization: Examples

- We have $b = -\frac{1}{2}A^T\lambda$ from the first “block row”
- Subsituting into $Ab = y$ (the second “block row”) yields $\lambda = -2(AA^T)^{-1}y$
- And hence

$$b = -\frac{1}{2}A^T\lambda = A^T(AA^T)^{-1}y$$

which was the solution we introduced (but didn’t derive) in Unit 1

Sequential Quadratic Programming

Sequential Quadratic Programming

- Consider equality constrained minimization

$$\min_{x\in\mathbb{R}^n} f(x) \quad \text{subject to} \quad g(x) = 0$$

  where $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$

- With the Lagrangian $\mathcal{L}(x, \lambda) = f(x) + \lambda^T g(x)$, the necessary condition for optimality is

$$\nabla\mathcal{L}(x, \lambda) = \begin{bmatrix} \nabla f(x) + J_g^T(x)\lambda \\ g(x) \end{bmatrix} = 0$$

- Once again, this is a nonlinear system of equations that can be solved using Newton's method

Sequential Quadratic Programming

- To derive the Jacobian of this system, we write

$$\nabla \mathcal{L}(x,\lambda) = \begin{bmatrix} \nabla f(x) + \sum_{k=1}^{m} \lambda_k \nabla g_k(x) \\ g(x) \end{bmatrix} \in \mathbb{R}^{n+m}$$

- Then we differentiate w.r.t to $x \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}^m$
- For $i = 1, \ldots, n$, we have

$$(\nabla \mathcal{L}(x,\lambda))_i = \frac{\partial f(x)}{\partial x_i} + \sum_{k=1}^{m} \lambda_k \frac{\partial g_k(x)}{\partial x_i}$$

- Differentiating w.r.t x_j, for $i, j = 1, \ldots, n$, gives

$$\frac{\partial}{\partial x_j}(\nabla \mathcal{L}(x,\lambda))_i = \frac{\partial^2 f(x)}{\partial x_i \partial x_j} + \sum_{k=1}^{m} \lambda_k \frac{\partial^2 g_k(x)}{\partial x_i \partial x_j}$$

Sequential Quadratic Programming

- The top-left $n \times n$ block of the Jacobian of $\nabla\mathcal{L}(x, \lambda)$ is

$$B(x, \lambda) = H_f(x) + \sum_{k=1}^{m} \lambda_k H_{g_k}(x) \in \mathbb{R}^{n\times n}$$

- Differentiating $(\nabla\mathcal{L}(x, \lambda))_i$ w.r.t λ_j, for $i = 1, \ldots, n$, $j = 1, \ldots, m$, gives

$$\frac{\partial}{\partial\lambda_j}(\nabla\mathcal{L}(x, \lambda))_i = \frac{\partial g_j(x)}{\partial x_i}$$

- The top-right $n \times m$ block of the Jacobian of $\nabla\mathcal{L}(x, \lambda)$ is

$$J_g(x)^T \in \mathbb{R}^{n\times m}$$

Sequential Quadratic Programming

- For $i = n+1, \ldots, n+m$, we have

$$(\nabla \mathcal{L}(x, \lambda))_i = g_i(x)$$

- Differentiating $(\nabla \mathcal{L}(x, \lambda))_i$ w.r.t x_j, for $i = n+1, \ldots, n+m$, $j = 1, \ldots, n$, gives

$$\frac{\partial}{\partial x_j}(\nabla \mathcal{L}(x, \lambda))_i = \frac{\partial g_i(x)}{\partial x_j}$$

- The bottom-left $m \times n$ block of the Jacobian of $\nabla \mathcal{L}(x, \lambda)$ is

$$J_g(x) \in \mathbb{R}^{m \times n}$$

- The final $m \times m$ bottom right block is zero ($g_i(x)$ does not depend on λ_j)

Sequential Quadratic Programming

- We have derived the following Jacobian matrix for $\nabla \mathcal{L}(x, \lambda)$

$$\begin{bmatrix} B(x, \lambda) & J_g^T(x) \\ J_g(x) & 0 \end{bmatrix} \in \mathbb{R}^{(m+n)\times(m+n)}$$

- Note the 2×2 block structure of this matrix
- Matrices with this structure are called KKT matrices after Karush, Kuhn, and Tucker

Sequential Quadratic Programming

- Therefore, Newton's method for $\nabla \mathcal{L}(x, \lambda) = 0$ is

$$\begin{bmatrix} B(x_k, \lambda_k) & J_g^T(x_k) \\ J_g(x_k) & 0 \end{bmatrix} \begin{bmatrix} s_k \\ \delta_k \end{bmatrix} = - \begin{bmatrix} \nabla f(x_k) + J_g^T(x_k)\lambda_k \\ g(x_k) \end{bmatrix}$$

  for $k = 0, 1, 2, \ldots$

- Here $(s_k, \delta_k) \in \mathbb{R}^{n+m}$ is the k-th Newton step

Sequential Quadratic Programming

- Now, consider the constrained minimization problem, where (x_k, λ_k) is our Newton iterate at step k:

$$\min_s \left\{ \frac{1}{2} s^T B(x_k, \lambda_k) s + s^T (\nabla f(x_k) + J_g^T(x_k)\lambda_k) \right\}$$

$$\text{subject to} \quad J_g(x_k)s + g(x_k) = 0$$

- The objective function is quadratic in s (here x_k, λ_k are constants)
- This minimization problem has Lagrangian

$$\begin{aligned} \mathcal{L}_k(s, \delta) = {} & \frac{1}{2} s^T B(x_k, \lambda_k) s + s^T (\nabla f(x_k) + J_g^T(x_k)\lambda_k) \\ & + \delta^T (J_g(x_k)s + g(x_k)) \end{aligned}$$

Sequential Quadratic Programming

- Then solving $\nabla \mathcal{L}_k(s, \delta) = 0$ (i.e. first-order necessary conditions) gives a linear system, which is the same as the k-th Newton step
- Therefore, at each step of Newton's method, we exactly solve a minimization problem with a quadratic objective and linear constraints
- Optimization of this type is called quadratic programming
- Therefore, Newton's method applied to $\mathcal{L}(x, \lambda) = 0$ is called sequential quadratic programming (SQP)

Sequential Quadratic Programming

- SQP is an important method, and there are many issues to be considered to obtain an efficient and reliable implementation:
  - efficient solution of the linear systems at each Newton iteration — matrix block structure can be exploited
  - quasi-Newton approximations to the Hessian
  - trust region, line search to improve robustness
  - treatment of constraints (equality and inequality) during the iterative process
  - selection of a good initial guess for λ

Penalty Methods

- Another approach to constrained optimization is penalty methods
- This converts a constrained problem into an unconstrained problem
- Key idea: Introduce a new objective function
  which is a weighted sum of objective function and constraints

Penalty Methods

- Given the minimization problem

$$\min_x f(x) \quad \text{subject to} \quad g(x) = 0$$

define the corresponding penalized unconstrained problem

$$\min_x \phi_\rho(x) = f(x) + \frac{1}{2}\rho g(x)^T g(x)$$

with a parameter $\rho \in \mathbb{R}$

- Let x^* be the solution of the constrained problem
- Let x_ρ^* be the solution of the penalized unconstrained problem
- Under appropriate conditions, it can be shown that

$$\lim_{\rho \to \infty} x_\rho^* = x^*$$

Penalty Methods

- In practice, we can solve the unconstrained problem for a large value of ρ to get a good approximation of x^*
- Another strategy is to solve for a sequence of penalty parameters ρ_k, where $x^*_{\rho_k}$ serves as an initial guess for $x^*_{\rho_{k+1}}$
- Note that the major drawback of penalty methods is that a large factor ρ will increase the condition number of the Hessian H_{ϕ_ρ}
- However, penalty methods can be convenient due to their simplicity

PDE-Constrained Optimization

PDE-Constrained Optimization

- Consider a general optimization problem

$$\min_{p \in \mathbb{R}^n} \mathcal{G}(p)$$

  with the objective function $\mathcal{G} : \mathbb{R}^n \to \mathbb{R}$
- Gradient-based methods require gradients of the objective
- They could be approximated with finite differences

PDE-Constrained Optimization

- However, each partial derivative requires an extra evaluation of $\mathcal{G}$

  $$\frac{\partial \mathcal{G}(p)}{\partial p_i} \approx \frac{\mathcal{G}(p + he_i) - \mathcal{G}(p)}{h},$$

  so we need $n+1$ evaluations of $\mathcal{G}$ to approximate $\nabla \mathcal{G}(p)$
- For example, if $\mathcal{G}(p)$ requires solving a PDE and parameters p represent an unknown field on a grid, this procedure becomes too expensive
- The accuracy of finite differences is also limited

PDE-Constrained Optimization

- There are two main alternative approaches for computing gradients of solutions of ODEs or PDEs
  - direct method
  - adjoint method
- The direct method is simpler, but the adjoint method is more efficient in cases with many parameters

One-Dimensional Case

- Consider the boundary value problem for an ODE

$$-u''(x;p) + r(x;p)u(x;p) = f(x), \qquad u(a) = u(b) = 0$$

  referred to as the primal equation
- Here the functions $r : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ and $f : \mathbb{R} \to \mathbb{R}$ are given
- The objective function $\mathcal{G} : \mathbb{R}^n \to \mathbb{R}$ is assumed to be a linear functional

$$\mathcal{G}(p) = \int_a^b \sigma(x)u(x;p)\mathrm{d}x$$

  for some given function $\sigma : \mathbb{R} \to \mathbb{R}$

Direct Method

- Note that the gradient of the objective is

$$\frac{\partial \mathcal{G}(p)}{\partial p_i} = \int_a^b \sigma(x) \frac{\partial u}{\partial p_i} \mathrm{d}x$$

  so we can compute it from derivatives of the solution $\frac{\partial u}{\partial p_i}$

- Differentiate the original ODE with respect to p_i

$$-\frac{\partial u}{\partial p_i}''(x;p) + r(x;p)\frac{\partial u}{\partial p_i}(x;p) = -\frac{\partial r}{\partial p_i} u(x;p)$$

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

Direct Method

- Once we compute each $\frac{\partial u}{\partial p_i}$ we can then evaluate $\nabla \mathcal{G}(p)$ by evaluating a sequence of n integrals
- This is not much better than using finite differences: we still need to solve n separate problems
- However, those can be cheaper since only the right-hand side changes. For example, we can reuse a common LU factorization

Adjoint Method

- A more efficient approach when n is large is the adjoint method
- The adjoint problem is defined as

$$-z''(x;p) + r(x;p)z(x;p) = \sigma(x), \qquad z(a) = z(b) = 0$$

- Since $\sigma(x)$ enters the right-hand side,
  the adjoint problem depends on the objective

Adjoint Method

- Given a solution $z(x;p)$ of the adjoint problem, the gradient is

$$\begin{aligned}\frac{\partial \mathcal{G}(p)}{\partial p_i} &= \int_a^b \sigma(x)\frac{\partial u}{\partial p_i}\mathrm{d}x \\ &= \int_a^b \left[-z''(x;p) + r(x;p)z(x;p)\right]\frac{\partial u}{\partial p_i}\mathrm{d}x \\ &= \int_a^b z(x;p)\left[-\frac{\partial u}{\partial p_i}''(x;p) + r(x;p)\frac{\partial u}{\partial p_i}(x;p)\right]\mathrm{d}x\end{aligned}$$

- The last line follows from integrating by parts twice (boundary terms vanish because $\frac{\partial u}{\partial p_i}$ and z are zero at a and b)

Adjoint Method

- Recall the derivative of the primal problem with respect to p_i

$$-\frac{\partial u}{\partial p_i}''(x;p) + r(x;p)\frac{\partial u}{\partial p_i}(x;p) = -\frac{\partial r}{\partial p_i}u(x;p)$$

- Combining both, we get

$$\frac{\partial \mathcal{G}(p)}{\partial p_i} = -\int_a^b \frac{\partial r}{\partial p_i} z(x;p)u(x;p)\mathrm{d}x$$

- Therefore, we only need to solve the primal and adjoint problems once and then can obtain each component of $\nabla\mathcal{G}(p)$ from the integral
- This idea extends to PDEs

Linear Programming

Linear Programming

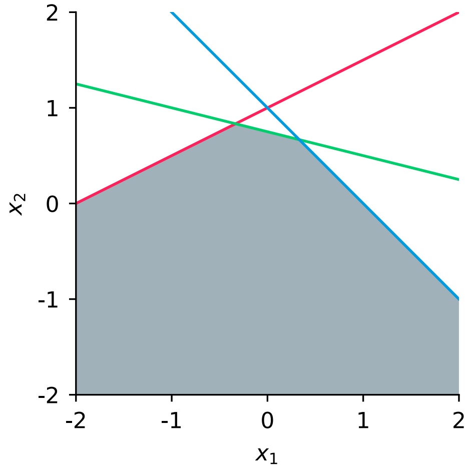
- As we mentioned earlier, the optimization problem

$$\min_{x\in\mathbb{R}^n} f(x) \text{ subject to } g(x) = 0 \text{ and } h(x) \leq 0,$$

  with f, g, h affine, is called a linear programming problem
- The feasible region is a convex polyhedron
- Since the objective function has a constant non-zero gradient, its global minimum must occur at a vertex of the feasible region

Linear Programming

- Example of a convex feasible region in $\mathbb{R}^2$



Linear Programming

- The standard approach to linear programming is conceptually simple: try a sequence of the vertices to find the minimum
- This is called the simplex method
- In the worst case, the computational cost of the simplex method grows exponentially with the size of the problem
- But this worst-case behavior is rare. In practice, the cost grows linearly
- We will not discuss the implementation of the simplex method

Linear Programming

- `scipy.optimize.linprog` uses the HiGHS library that implements the dual revised simplex method
- See [examples/unit4/linprog.py], solving the problem

$$\min_{x} f(x) = -5x_1 - 4x_2 - 6x_3$$

subject to

$$\begin{aligned} x_1 - x_2 + x_3 &\leq \quad 20 \\ 3x_1 + 2x_2 + 4x_3 &\leq \quad 42 \\ 3x_1 + 2x_2 &\leq \quad 30 \end{aligned}$$

and $0 \leq x_1, 0 \leq x_2, 0 \leq x_3$