AM 205: lecture 19

- Last time: Conditions for optimality
- Today: Newton's method for optimization, survey of optimization methods

Newton's Method

Python example: Newton's method for minimization of Himmelblau's function

$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$

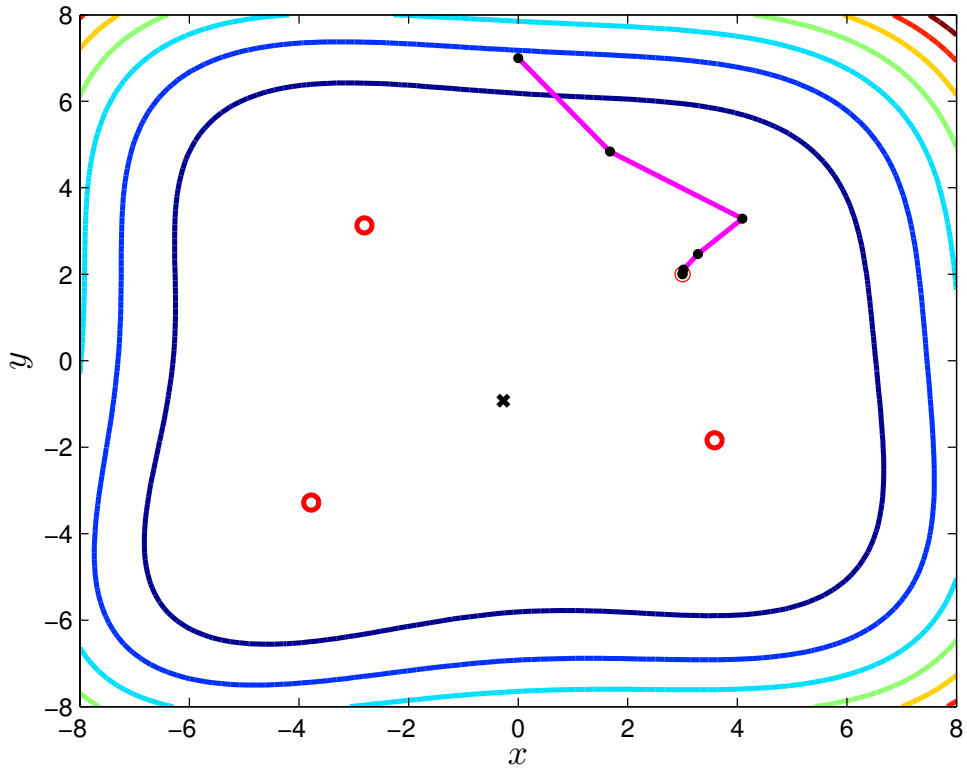
Local maximum of 181.617 at $(-0.270845, -0.923039)$

Four local minima, each of 0, at

$$(3, 2),\ (-2.805, 3.131),\ (-3.779, -3.283),\ (3.584, -1.841)$$

Newton's Method

Python example: Newton's method for minimization of Himmelblau's function



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 max. as can happen with raw Newton method

The line search modifies the Newton step size, hence 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 $\|x_{k+1} - x_k\| \leq R_k$, hence 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

Newton's method is effective for optimization, but it can be unreliable, expensive, and complicated

- Unreliable: Only converges when sufficiently close to a minimum
- Expensive: The Hessian H_f is dense in general, hence very expensive if n is large
- Complicated: Can be impractical or laborious to derive the Hessian

Hence there has been much interest in so-called quasi-Newton methods, which do not require the Hessian

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 superlinear convergence is achieved

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 Hessian guess, *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

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

BFGS

See lecture: derivation of the Broyden root-finding algorithm

See lecture: derivation of the BFGS algorithm

Basic idea is that B_k accumulates second derivative information on successive iterations, eventually approximates H_f well

BFGS

Actual implementation of BFGS: store and update inverse Hessian to avoid solving linear system:

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

where

$$\Delta H_k \equiv (I - s_k \rho_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T, \qquad \rho_k = \frac{1}{y_k^T s_k}$$

BFGS

BFGS is implemented as the `fmin_bfgs` function in `scipy.optimize`

Also, BFGS (+ trust region) is implemented in Matlab's `fminunc` function, *e.g.*

```
x0 = [5;5];
options = optimset('GradObj','on');
[x,fval,exitflag,output] = ...
  fminunc(@himmelblau_function,x0,options);
```

Conjugate Gradient Method

The conjugate gradient (CG) method is another alternative to Newton's method that does not require the Hessian:

1: choose initial guess x_0
2: $g_0 = \nabla f(x_0)$
3: $x_0 = -g_0$
4: **for** $k = 0, 1, 2, \ldots$ **do**
5: choose η_k to minimize $f(x_k + \eta_k s_k)$
6: $x_{k+1} = x_k + \eta_k s_k$
7: $g_{k+1} = \nabla f(x_{k+1})$
8: $\beta_{k+1} = (g_{k+1}^T g_{k+1})/(g_k^T g_k)$
9: $s_{k+1} = -g_{k+1} + \beta_{k+1} s_k$
10: **end for**

Constrained Optimization

Equality Constrained Optimization

We now 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 $\mathcal{L}(x, \lambda) = f(x) + \lambda^T g(x)$, we recall from that 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 via 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 need to differentiate wrt 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 wrt 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

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

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

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

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

Hence 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 $(\nabla \mathcal{L}(x, \lambda))_i$ wrt x_j, for $i = n+1, \ldots, n+m$, $j = 1, \ldots, n$, gives

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

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

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

. . . and the final $m \times m$ bottom right block is just zero (differentiation of $g_i(x)$ w.r.t. λ_j)

Sequential Quadratic Programming

Hence, 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 often called KKT matrices[1])

[1] Karush, Kuhn, Tucker: did seminal work on nonlinear optimization

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

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

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 kth Newton step

Hence at each step of Newton's method, we exactly solve a minimization problem (quadratic objective fn., linear constraints)

An optimization problem of this type is called a quadratic program

This motivates the name for applying Newton's method to $\mathcal{L}(x, \lambda) = 0$: 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 (as in the unconstrained case)
- Trust region, line search etc to improve robustness
- Treatment of constraints (equality and inequality) during the iterative process
- Selection of good starting guess for λ

Penalty Methods

Another computational strategy for constrained optimization is to employ 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 constraint

Penalty Methods

Given the minimization problem

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

we can consider the related unconstrained problem

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

Let x^* and x_ρ^* denote the solution of $(*)$ and $(**)$, respectively

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 a starting 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}

On the other hand, penalty methods can be convenient, primarily due to their simplicity

Linear Programming

Linear Programming

As we mentioned earlier, the optimization problem

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

with f, g, h affine, is called a linear program

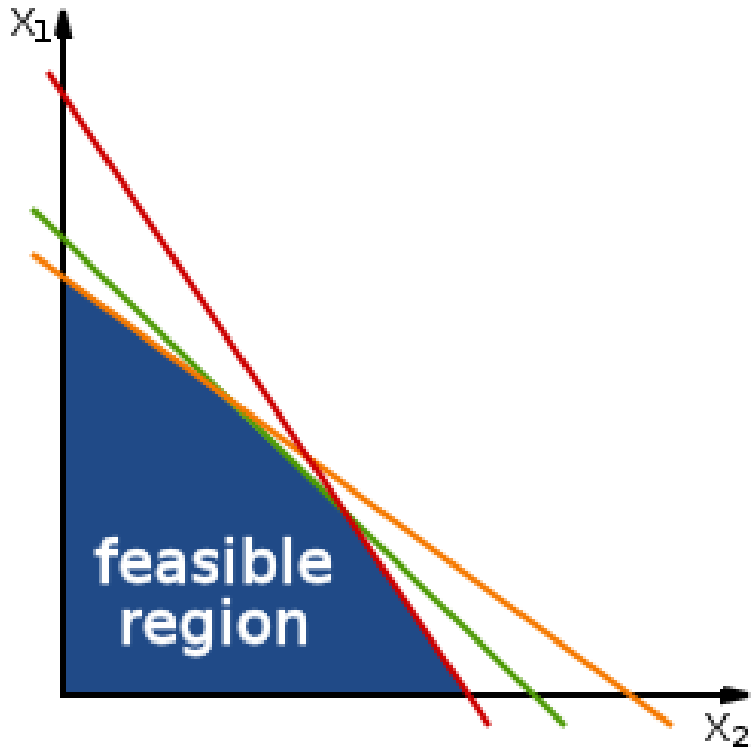
The feasible region is a convex polyhedron[2]

Since the objective function maps out a hyperplane, its global minimum must occur at a vertex of the feasible region

[2] Polyhedron: a solid with flat sides, straight edges

Linear Programming

This can be seen most easily with a picture (in $\mathbb{R}^2$)



Linear Programming

The standard approach for solving linear programs is conceptually simple: examine a sequence of the vertices to find the minimum

This is called the simplex method

Despite its conceptual simplicity, it is non-trivial to develop an efficient implementation of this algorithm

We will not discuss the implementation details of the simplex method...

Linear Programming

In the worst case, the computational work required for the simplex method grows exponentially with the size of the problem

But this worst-case behavior is extremely rare; in practice simplex is very efficient (computational work typically grows linearly)

Newer methods, called interior point methods, have been developed that are polynomial in the worst case

Nevertheless, simplex is still the standard approach since it is more efficient than interior point for most problems

Linear Programming

Python example: Using `cvxopt`, solve the linear program

$$\min_x f(x) = -5x_1 - 4x_2 - 6x_3$$

subject to

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

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

(LP solvers are efficient, main challenge is to formulate an optimization problem as a linear program in the first place!)

PDE Constrained Optimization

PDE Constrained Optimization

We will now consider optimization based on a function that depends on the solution of a PDE

Let us denote a parameter dependent PDE as

$$\text{PDE}(u(p); p) = 0$$

- $p \in \mathbb{R}^n$ is a parameter vector; could encode, for example, the flow speed and direction in a convection–diffusion problem
- $u(p)$ is the PDE solution for a given p

PDE Constrained Optimization

We then consider an output functional g,[3] which maps an arbitrary function v to $\mathbb{R}$

And we introduce a parameter dependent output, $\mathcal{G}(p) \in \mathbb{R}$, where $\mathcal{G}(p) \equiv g(u(p)) \in \mathbb{R}$, which we seek to minimize

At the end of the day, this gives a standard optimization problem:

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

[3] A functional is just a map from a vector space to $\mathbb{R}$

PDE Constrained Optimization

One could equivalently write this PDE-based optimization problem as

$$\min_{p,u} g(u) \quad \text{subject to} \quad \text{PDE}(u; p) = 0$$

For this reason, this type of optimization problem is typically referred to as PDE constrained optimization

- objective function g depends on u
- u and p are related by the PDE constraint

Based on this formulation, we could introduce Lagrange multipliers and proceed in the usual way for constrained optimization ...