Nonlinear Programming 2

- Unconstrained Optimization 1: line search, search interval, extreme values of convex functions, smooth and nonsmooth line search
- Unconstrained Optimization 2: multivariable unconstrained optimization, steepest descent method
- Solving a constrained nonlinear program using unconstrained optimization: exterior penalty function methods, (interior) barrier function methods, choosing penalty and barrier functions, comparison, examples

Recall: Feasible Directions

- Given a nonlinear program $\min f(\boldsymbol{x}) : \boldsymbol{x} \in X$, where $X = \{ \boldsymbol{x} : g_i(\boldsymbol{x}) \leq 0, i \in \{1, \dots, m\} \}$ and f and g_i are smooth (continuously differentiable) functions on X
- We use the fact that if \bar{x} is a local minimum then there is no (improving) feasible direction d at \bar{x} and $\delta > 0$ so that

$$\forall \lambda \in (0, \delta) : \quad f(\bar{\boldsymbol{x}} + \lambda \boldsymbol{d}) < f(\bar{\boldsymbol{x}})$$

 $\bar{\boldsymbol{x}} + \lambda \boldsymbol{d} \in X$

- Only necessary, but for convex programs also sufficient (subject to certain constraint qualifications we do not discuss here)
- We solve the nonlinear program by iteratively moving along feasible directions

Recall: Feasible Directions

- Seek a point where there is no improving feasible direction
- Let $J \subseteq I$ be the set of tight constraints at \bar{x}

$$\forall i \in J : g_i(\bar{\boldsymbol{x}}) = 0, \quad \forall i \in I \setminus J : g_i(\bar{\boldsymbol{x}}) < 0$$

• An improving feasible direction is the below (if exists):

$$\boldsymbol{d}: \nabla f(\bar{\boldsymbol{x}})^T \boldsymbol{d} < 0, \ \nabla g_i(\bar{\boldsymbol{x}})^T \boldsymbol{d} < 0 \quad \forall i \in J$$

• We can find such *d* by solving the below problem:

 $z_{opt} = \min \nabla f(\bar{\boldsymbol{x}})^T \boldsymbol{d} : |\boldsymbol{d}| \le 1, \ \nabla g_i(\bar{\boldsymbol{x}})^T \boldsymbol{d} < 0 \quad \forall i \in J$

- Linear objective function, linear (linearizable) constraints
- Successive linear programming

Recall: Line Search

- If $z_{opt} \sim 0$ then \bar{x} is (probably) a local minimum: in some pathological cases the condition might not be sufficient
- If $z_{opt} < 0$ then d is an improving feasible direction
- Line search along the ray x
 - λd : λ > 0 so that
 • the feasible region is not left and
 - $\circ\;$ the objective function is minimized along d
- Simple nonlinear program with a single unknown, where the feasible region is an interval (or the entire \mathbb{R})

$$\min f(\bar{\boldsymbol{x}} + \lambda \boldsymbol{d}) : \bar{\boldsymbol{x}} + \lambda \boldsymbol{d} \in X, \lambda \ge 0$$

- Interior point methods often work this way: find a "good" direction and perform line search to find the ideal step size
- We need an efficient algorithm to perform line search

Line Search

- Find the optimal solution of the optimization problem $\min \theta(\lambda) : \lambda \in [a, b]$ where θ is **convex** and **smooth**
- We concentrate on convex functions: the ideas can be generalized to the nonconvex case as well
- We rely on the assumption that θ is differentiable: for the convex nonsmooth case, one can use dichotomous search for instance
- The interval [a, b] is called the **search interval**

• **Theorem:** a smooth function f is convex on some set X if and only if

$$\forall \boldsymbol{x}, \boldsymbol{y} \in X: \quad f(\boldsymbol{y}) \ge f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\boldsymbol{y} - \boldsymbol{x})$$
 (1)

Geometrically: the tangent space at x bounds f from below



• Useful for outer linearization: approximating a nonlinear constraint system $X = \{ \boldsymbol{x} : g_i(\boldsymbol{x}) \le 0, i = 1, ..., m \}$ at $\bar{\boldsymbol{x}}$ with $\bar{X} = \{ \boldsymbol{x} : g_i(\bar{\boldsymbol{x}}) + \nabla g_i(\bar{\boldsymbol{x}})^T (\boldsymbol{x} - \bar{\boldsymbol{x}}) \le 0, i = 1, ..., m \}$

- **Proof:** supposing first that *f* is convex, we show that (1) holds
- *f* is convex: the line segment between f(x) and f(y) upper bounds the function of *f* between points x and y

$$\forall \lambda \in [0,1] : f(\lambda \boldsymbol{y} + (1-\lambda)\boldsymbol{x}) \le \lambda f(\boldsymbol{y}) + (1-\lambda)f(\boldsymbol{x})$$

• Using that $\mu a + (1 - \mu)b = b + \mu(a - b)$:

$$f(\boldsymbol{x} + \lambda(\boldsymbol{y} - \boldsymbol{x})) \leq f(\boldsymbol{x}) + \lambda(f(\boldsymbol{y}) - f(\boldsymbol{x}))$$

• Bringing $f(\boldsymbol{x})$ to the left-hand side and dividing by λ :

$$\frac{f(\boldsymbol{x} + \lambda(\boldsymbol{y} - \boldsymbol{x})) - f(\boldsymbol{x})}{\lambda} \le f(\boldsymbol{y}) - f(\boldsymbol{x})$$

• Taking the limit $\lambda \to 0$ gives the desired inequality:

$$\nabla f(\boldsymbol{x})^T(\boldsymbol{y}-\boldsymbol{x}) \leq f(\boldsymbol{y}) - f(\boldsymbol{x})$$

since the directional derivative of f in the direction $(\boldsymbol{y} - \boldsymbol{x})$:

$$\lim_{\lambda \to 0} \frac{f(\boldsymbol{x} + \lambda(\boldsymbol{y} - \boldsymbol{x})) - f(\boldsymbol{x})}{\lambda} = \nabla^T f(\boldsymbol{x})(\boldsymbol{y} - \boldsymbol{x})$$

- In the other direction: we show that from (1) the convexity of *f* follows
- Let $x_1, x_2 \in X$ by two arbitrary points in X and let x be a convex combination of x_1 and x_2

$$\boldsymbol{x} = \lambda \boldsymbol{x}_1 + (1 - \lambda) \boldsymbol{x}_2, \quad \lambda \in [0, 1]$$

• First, write (1) for the case when $oldsymbol{y} = oldsymbol{x}_1$

$$f(\boldsymbol{x}_1) \ge f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\boldsymbol{x}_1 - \boldsymbol{x})$$
(2)

• Second, write (1) for the case when $oldsymbol{y} = oldsymbol{x}_2$

$$f(\boldsymbol{x}_2) \geq f(\boldsymbol{x}) +
abla f(\boldsymbol{x})^T (\boldsymbol{x}_2 - \boldsymbol{x})$$
 (3)

• Multiply (2) by λ and (3) by $1 - \lambda$ and sum the two:

$$\lambda f(\boldsymbol{x}_1) \ge \lambda f(\boldsymbol{x}) + \lambda \nabla f(\boldsymbol{x})^T (\boldsymbol{x}_1 - \boldsymbol{x})$$
$$(1 - \lambda) f(\boldsymbol{x}_2) \ge (1 - \lambda) f(\boldsymbol{x}) + (1 - \lambda) \nabla f(\boldsymbol{x})^T (\boldsymbol{x}_2 - \boldsymbol{x})$$

 $\lambda f(\boldsymbol{x}_1) + (1-\lambda)f(\boldsymbol{x}_2) \ge f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2 - \boldsymbol{x})$

• Since $m{x}$ is a convex combination of $m{x}_1$ and $m{x}_2$ we can:

 $\circ~$ on the right-hand side substitute $f({\boldsymbol x})$ with

$$f(\lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2)$$

 \circ rewrite the gradient for the expression in parentheses:

$$egin{aligned} \lambda oldsymbol{x}_1 + (1-\lambda)oldsymbol{x}_2 - oldsymbol{x} = \ \lambda oldsymbol{x}_1 + (1-\lambda)oldsymbol{x}_2 - (\lambda oldsymbol{x}_1 + (1-\lambda)oldsymbol{x}_2) = 0 \end{aligned}$$

• We obtain precisely the definition of convexity of f:

$$\lambda f(\boldsymbol{x}_1) + (1-\lambda)f(\boldsymbol{x}_2) \ge f(\lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2)$$

- Holds for any x_1 , x_2 , and x, which concludes the proof
- One of the cornerstone theorems of convex analysis

- Corollary: given f be smooth and convex and $\bar{x} \in \mathbb{R}^n$, $f(\bar{x})$ is a global minimum of f if and only if $\nabla f(\bar{x}) = 0$
- **Proof:** earlier, we have seen that $\nabla f(\bar{x}) = 0$ is necessary for $f(\bar{x})$ to be a minimum
- In the general case $\nabla f(\bar{x}) = 0$ is not sufficient though (it also holds at inflection points, saddle points, etc.)
- For convex functions, however, it is also sufficient
- To see this, suppose $\nabla f(\bar{x}) = 0$ and use the previous theorem for \bar{x} and arbitrary y:

$$f(\boldsymbol{y}) \ge f(\bar{\boldsymbol{x}}) + \nabla f(\bar{\boldsymbol{x}})^T (\boldsymbol{y} - \bar{\boldsymbol{x}}) = f(\bar{\boldsymbol{x}}) + 0$$

• So $f(\bar{\boldsymbol{x}})$ is a global minimum

- In single dimension, the finding extreme values is much simpler
- A function $\theta(\lambda) : \mathbb{R} \mapsto \mathbb{R}$ is convex if and only if

$$\forall \mu, \nu : \quad \theta(\mu) \ge \theta(\nu) + \theta'(\nu)(\mu - \nu) \tag{4}$$

- For finding the minimum, simply find $\lambda: \theta'(\lambda) = 0$
- We can find the minimum for a smooth convex function efficiently using the above two results
- We can use simple binary search for finding $\lambda : \theta'(\lambda) = 0$ and it is enough to evaluate θ only once in each iteration

- Solve $\min \theta(\lambda) : \lambda \in [a, b]$, where θ is a smooth convex function on the search interval [a, b]
- Take any point $\lambda \in [a, b]$ and evaluate $\theta'(\lambda)$ -t
- One of three cases can occur:
 - $\circ \ \theta'(\lambda) = 0$: by the above, θ attains the minimum at λ
 - $\theta'(\lambda) > 0$: for any $\forall \mu > \lambda : \theta'(\lambda)(\mu \lambda) > 0$, so by (4) we obtain $\theta(\mu) > \theta(\lambda)$ and therefore the minimum cannot occur in the interval $[\lambda, b]$ and thus the search interval can be narrowed down to $[a, \lambda]$
 - $\theta'(\lambda) < 0$: just the opposite, $\forall \mu < \lambda : \theta(\mu) > \theta(\lambda)$ since $\theta'(\lambda)(\mu \lambda) > 0$ by $\theta'(\lambda) < 0$ and $\mu \lambda < 0$, and the new search interval is $[\lambda, b]$

- Choose λ so that the narrowed down search interval $\max{\{\lambda a, b \lambda\}}$ is minimal in the worst-case
- It is easy to see that this occurs at the middle point $\lambda = \frac{1}{2}(a+b)$ of the interval [a,b]
- Simple binary search:
 - $\circ~$ Initialization: choose search precision l>0, let $a_1=a,$ $b_1=b,$ and let k=1
 - 1. let $\lambda_k = \frac{1}{2}(a_k + b_k)$ and evaluate $\theta'(\lambda_k)$
 - 2. if $\theta'(\lambda) = 0$ or $b_k a_k < l$ then halt: the minimum occurs in the interval $[a_k, b_k]$
 - 3. if $\theta'(\lambda) > 0$ then $a_{k+1} = a_k$ and $b_{k+1} = \lambda_k$, otherwise $a_{k+1} = \lambda_k$ and $b_{k+1} = b_k$, and go to step (1)

- The size of the search interval at step k: $\frac{1}{2^k}(b-a)$
- The number of steps to reach precision $l: k \ge \log_2 \frac{b-a}{l}$
- Example: find the minimum of the function $\theta(\lambda) = \lambda^2 + 2\lambda$ on the interval [-5, 15] with precision $l = 2 \cdot 10^{-2}$
- We seek λ that satisfies $\theta'(\lambda) = 2\lambda + 2 = 0$, but very often the algebraic equation $\theta'(\lambda) = 0$ cannot be solved directly
- Using our numeric method (binary search) instead:

k	a	b	λ	$ heta^{\prime}(\lambda)$	$ heta(\lambda)$	b-a
1	-5.0000	15.0000	5.0000	12.0000	35.0000	20.0000
2	-5.0000	5.0000	0.0000	2.0000	0.0000	10.0000
3	-5.0000	0.0000	-2.5000	-3.0000	1.2500	5.0000
11	-1.0156	-0.9961	-1.0059	0.0118	-1.0000	0.0195

Unconstrained Optimization

- In practice we often need to move beyond single-dimension line search and minimize multivariable $\mathbb{R}^n \mapsto \mathbb{R}$ functions
- Given a nonlinear program $\min f(\boldsymbol{x}) : \boldsymbol{x} \in X$, let $X = \mathbb{R}^n$
- Suppose that *f* is smooth and convex
- The minimum occurs at point $\bar{\boldsymbol{x}}$ where $\nabla f(\bar{\boldsymbol{x}}) = \boldsymbol{0}$
- Usually this cannot be solved analytically, we need numeric methods and approximations
- We already have a method to optimize convex programs: the method of feasible directions due to Zoutendijk
- Much simpler in our case since now all directions are feasible $(X = \mathbb{R}^n)$
- We only need to take care of ensuring that the direction we find be improving

The Steepest Descent Method

- Some d is an improving direction at \bar{x} if $\nabla f(\bar{x})^T d < 0$
- Steepest descent: the unit vector \hat{d} moving along which we experience the largest drop in the value of f

• Theorem:
$$\underset{\hat{d}:\|\hat{d}\|=1}{\operatorname{argmin}} \nabla f(\bar{x})^T \hat{d} = -\frac{\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|}$$

• **Proof:** using the Cauchy–Schwarz Inequality and $\|\hat{d}\| = 1$:

$$\nabla f(\bar{\boldsymbol{x}})^T \hat{\boldsymbol{d}} \ge - \| \nabla f(\bar{\boldsymbol{x}}) \| \| \hat{\boldsymbol{d}} \| \ge - \| \nabla f(\bar{\boldsymbol{x}}) \|$$

- Holds with equality if and only if $\hat{d} = rac{abla f(ar{m{x}})}{\|
 abla f(ar{m{x}})\|}$
- So the best improving direction is $\hat{d} = rac{abla f(ar{x})}{\|
 abla f(ar{x})\|}$, then we can again use line search to find the ideal step size along \hat{d}

The Steepest Descent Method

- Solve the unconstrained nonlinear optimization problem $\min f(x) : x \in \mathbb{R}^n$ where f is smooth and convex
- Initialization: choose precision $\epsilon>0$ and x_1 initial point, and let k=1
- 1 Of $\|\nabla f(\boldsymbol{x}_k)\| < \epsilon$ then halt, \boldsymbol{x}_k is minimal
- 2 Otherwise $\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)$
- 3 Line search: solve the unconstrained search problem

$$\lambda_k = \min f(\boldsymbol{x}_k + \lambda \boldsymbol{d}_k) : \lambda \ge 0$$

4 Let $oldsymbol{x}_{k+1} = oldsymbol{x}_k + \lambda_k oldsymbol{d}_k$ and go to step (2)

The Steepest Descent Method

• Simple and, theoretically, it converges in finite steps, but hardly usable in practice due to zig-zagging



• Higher-order methods can avoid this: Newton's method, conjugate gradient, etc.

Penalty and Barrier Functions

- We have seen that constraints make the optimization much more difficult: improving directions are easy to find, feasible directions may be more difficult
- It would be nice to trace back constrained nonlinear programming to unconstrained optimization
- The idea is to enforce constraints via the objective function, by adding a term to the objective to penalize any violation of the constraints and to remove the constraints themselves
- Minimization of the resultant unconstrained problem will try to remove the penalty and thereby to satisfy the constraints
 - (exterior) penalty functions: infeasible points are penalized, the further the point from the feasible region the larger the penalty
 - (interior) barrier functions: even approaching the boundary of the feasible region already carries a penalty

• Consider the simple constrained nonlinear optimization problem

 $\min f(\boldsymbol{x}): h(\boldsymbol{x}) = 0$

where f and h are $\mathbb{R}^n \mapsto \mathbb{R}$ functions and $\boldsymbol{x} \in \mathbb{R}^n$

• Replace this constrained problem with the below unconstrained one:

$$\min f(\boldsymbol{x}) + \mu h^2(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^n$$

where $\mu>0$ is some large scalar

- Intuitively, at optimum the (external) penalty function $\mu h^2(x)$ will take a value close to zero, otherwise the penalty would prohibitively increase the objective value
- Choosing μ large enough ensures that the minimum of the original problem and the unconstrained problem coincide

• Nonlinear programs containing inequality constraints need a different penalty function

 $\min f(\boldsymbol{x}) : g(\boldsymbol{x}) \le 0$

- The penalty function $\mu g^2(x)$ would not work since it would penalize both g(x) < 0 and g(x) > 0 whereas we need to penalize only the latter
- Consider the below unconstrained problem instead:

$$\min f(\boldsymbol{x}) + \mu \max\{0, g(\boldsymbol{x})\} : \boldsymbol{x} \in \mathbb{R}^n$$

- Penalty is applied only if g(x) > 0, since for g(x) < 0 the penalty disappears by $\max\{0, g(x)\} = 0$
- Even better penalty function is $\mu(\max\{0, g(\boldsymbol{x})\})^2$: smooth!

• For the generic case when the nonlinear program contains both equality and inequality constraints:

$$\min f(\boldsymbol{x})$$
s.t. $g_i(\boldsymbol{x}) \le 0$ $i \in \{1, \dots, m\}$
 $h_i(\boldsymbol{x}) = 0$ $i \in \{1, \dots, n\}$

• The external penalty functions:

$$\alpha(\boldsymbol{x}) = \sum_{i=1}^{m} \Phi(g_i(\boldsymbol{x})) + \sum_{i=1}^{n} \Psi(h_i(\boldsymbol{x}))$$
$$\Phi(y) = (\max\{0, y\})^p, \quad \Psi(y) = |y|^p$$

for some p > 0 integer

• We obtain the below unconstrained nonlinear program:

$$\min f(\boldsymbol{x}) + \mu \left(\sum_{i=1}^{m} \left(\max\{0, g_i(\boldsymbol{x})\} \right)^p + \sum_{i=1}^{n} |h_i(\boldsymbol{x})|^p \right) :$$
$$\boldsymbol{x} \in \mathbb{R}^n$$

- Can be solved using the unconstrained optimization methods discussed previously
- Can be started from arbitrary, even from an infeasible point
- Drawback is that the search enters into the feasible region only in the vicinity of the optimum, exactly where zig-zagging is most prominent
- Large μ needed for reliable result: numeric instability

Penalty Function Methods: Example

• Consider the constrained (non)linear program

$$\min x \\ \text{s.t.} \quad -x+2 \le 0$$

- Optimum at $\bar{x} = 2$: $f(\bar{x}) = 2$
- Solve the problem using penalty functions
- Using the penalty function $\alpha(x) = (\max\{0, g(x)\})^2$ the constrained problem as an unconstrained nonlinear program:

$$\alpha(x) = \begin{cases} 0 & \text{ha } x \geq 2\\ (-x+2)^2 & \text{ha } x < 2 \end{cases}$$

Penalty Function Methods: Example

- $\alpha(x)$ $f(x) + \mu \alpha(x)$ 2 ()
 - $f(x) + \mu \alpha(x)$ is convex, so we can find the minimum easily
 - The derivative for x < 2:

 $(f(x) + \mu\alpha(x))' = 1 + 2\mu(x - 2) = 0$

• The optimal solution:

$$\overline{x} = 2 - \frac{1}{2\mu}$$

- Approximates the real optimum as $\mu \to \infty$
- x In general, guaranteed to converge in finite steps

Penalty Function Methods: Example

Solve the constrained optimization problem

$$\min x_1^2 + x_2^2 : x_1 + x_2 - 1 = 0$$

- Optimal solution: $\begin{bmatrix} x_1 & x_2 \end{bmatrix}^T = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^T$, optimum: $\frac{1}{2}$
- Apply the penalty function $\alpha(y) = |y|^2$:

$$\min x_1^2 + x_2^2 + \mu(x_1 + x_2 - 1)^2 : x_1, x_2 \in \mathbb{R}$$

• Convex for $\forall \mu \geq 0$, so the minimum occurs where:

$$2x_1 + 2\mu(x_1 + x_2 - 1) = 0$$
$$2x_2 + 2\mu(x_1 + x_2 - 1) = 0$$

– p. 27

• From the two equations: $x_1 = x_2 = \frac{1}{2 + \frac{1}{\mu}}$, optimal if $\mu \to \infty$

Barrier Function Methods

- External penalty function methods converge through a sequence of infeasible points
- Internal barrier functions do not allow the search to leave the feasible region in the first place
- Given a linear program with inequality constraints:

min $f(\boldsymbol{x})$ s.t. $g_i(\boldsymbol{x}) \le 0$ $i \in \{1, \dots, m\}$

• Instead, solve the unconstrained problem

 $\min f(\boldsymbol{x}) + \mu \beta(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^n$

Barrier Function Methods

 The internal barrier function β takes nonnegative values in the interior of the feasible region and tends to infinity at the boundary:

$$\beta(\boldsymbol{x}) = \sum_{i=1}^{m} \Phi(g_i(\boldsymbol{x}))$$

where barrier function Φ has the following properties:

$$\Phi(y) \ge 0 \text{ if } y < 0, \qquad \lim_{y \to 0^-} \Phi(y) = \infty$$

- The barrier function prohibits passing the boundary of the feasible region
- Equality conditions are more involving to handle here

Barrier Function Methods

• Typical internal barrier functions:

$$eta(oldsymbol{x}) = \sum_{i=1}^m rac{-1}{g_i(oldsymbol{x})}, \qquad eta(oldsymbol{x}) = -\sum_{i=1}^m \ln\left(\min\left\{1, -g_i(oldsymbol{x})
ight\}
ight)$$

- The augmented objective function can be optimized using unconstrained methods and we never step out of the feasible region
- Drawback is that the penalty appears even at the optimum and the optimum cannot occur at a boundary point
- Plus the iteration must start from a feasible point, otherwise we never get to the other "good" side of the barrier
- Works reliably when μ is small, but too small value for μ again causes numerical instability and badly conditioned problems

Barrier Function Methods: Example

• Consider the nonlinear program

$$\begin{array}{l} \min \ x \\ \text{s.t.} \ -x+1 \le 0 \end{array}$$

- The optimum is 1, attained by the objective at $\bar{x} = 1$
- Let the internal barrier function be as follows:

$$\beta(x) = \frac{-1}{-x+1} = \frac{1}{x-1} \qquad x \neq 1$$

• The resultant unconstrained problem:

$$\min x + \frac{\mu}{x-1} : x \in \mathbb{R}$$

Barrier Function Methods: Example

- Solving $\min x + \frac{\mu}{x-1} : x \in \mathbb{R}$ only makes sense of x > 1, we need to take care of this ourselves
- The objective function is convex, the minimum occurs at $\frac{d}{dx}(f(x) + \mu\beta(x)) = 0$ from which we obtain $\bar{x} = 1 + \sqrt{\mu}$, optimal for $\mu \to 0$

