

Lecture 13

Feasible direction methods

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- ▶ Consider the problem to find

$$f^* = \text{infimum } f(x), \quad (1a)$$

$$\text{subject to } x \in X, \quad (1b)$$

$X \subseteq \mathbb{R}^n$ nonempty, **closed & convex**; $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is C^1 on X

- ▶ Solution idea: generalize unconstrained optimization methods

- Step 0.** Determine a *starting point* $x_0 \in X$. Set $k := 0$
- Step 1.** Find a *feasible descent search direction* $p_k \in \mathbb{R}^n$, such that there exists $\bar{\alpha} > 0$ satisfying
- ▶ $x_k + \alpha p_k \in X, \forall \alpha \in (0, \bar{\alpha}]$
 - ▶ $f(x_k + \alpha p_k) < f(x_k), \forall \alpha \in (0, \bar{\alpha}]$
- Step 2.** Determine a *step length* $\alpha_k > 0$ such that $f(x_k + \alpha_k p_k) < f(x_k)$ and $x_k + \alpha_k p_k \in X$
- Step 3.** Let $x_{k+1} := x_k + \alpha_k p_k$
- Step 4.** If a *termination criterion* is fulfilled, then stop!
Otherwise, let $k := k + 1$ and go to Step 1

- ▶ Just as **local** as methods for unconstrained optimization
- ▶ Search direction often of the form $p_k = y_k - x_k$, where $y_k \in X$ solves an (easy) approximate problem
- ▶ Line searches analogous to unconstrained case
- ▶ Termination criteria and descent based on first-order optimality and/or fixed-point theory ($p_k \approx 0^n$)

- ▶ For general X , finding feasible descent direction and step length is difficult (e.g., systems of nonlinear equations)
- ▶ X polyhedral \implies search directions and step length easy to find
- ▶ X polyhedral \implies local minima are KKT points
- ▶ Methods (to be discussed) will find KKT points

- ▶ Frank–Wolfe method based on first-order approximation of f at x_k :

- ▶ First-order (necessary) optimality conditions:

$$x^* \text{ local minimum of } f \text{ on } X \implies \nabla f(x^*)^T(x - x^*) \geq 0, \quad x \in X$$

$$x^* \text{ local minimum of } f \text{ on } X \implies \underset{x \in X}{\text{minimize}} \quad \nabla f(x^*)^T(x - x^*) = 0$$

- ▶ Satisfying necessary conditions $\not\Rightarrow$ x^* local minimum
- ▶ Violate necessary conditions \Rightarrow can construct feasible descent dir.

- ▶ At iterate $x_k \in X$, if

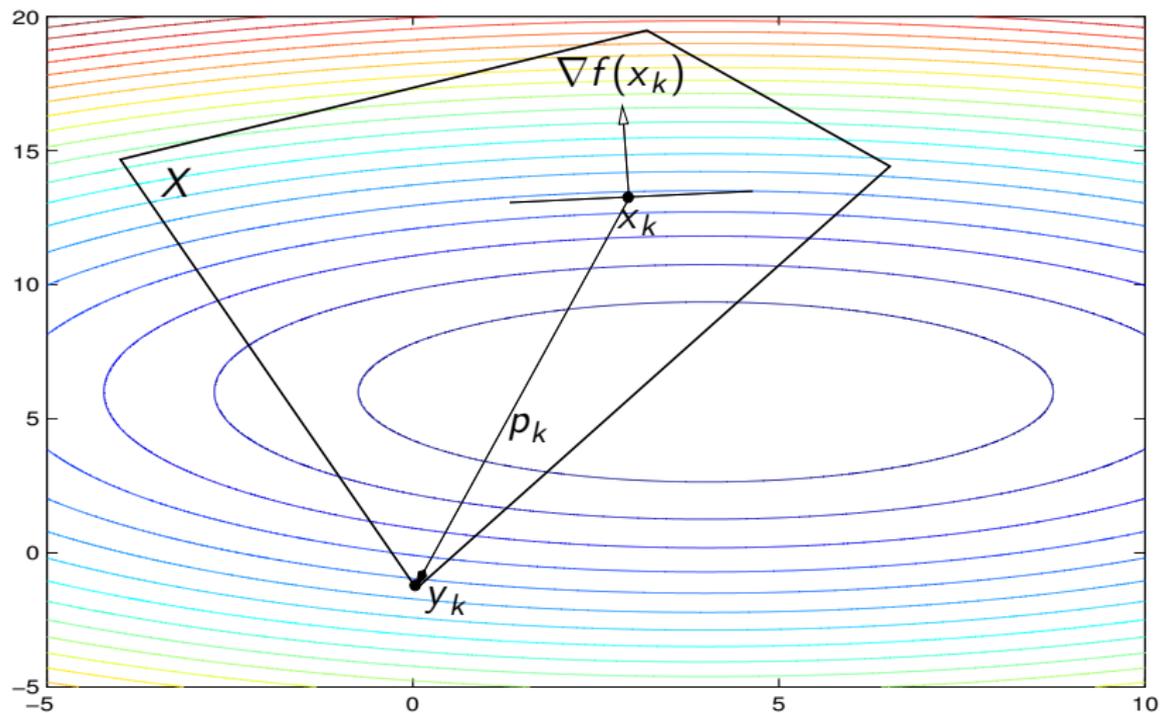
$$\begin{cases} \text{minimize}_{y \in X} \nabla f(x_k)^T (y - x_k) < 0, \\ y_k \in \operatorname{argmin}_{y \in X} \nabla f(x_k)^T (y - x_k) \end{cases}$$

Then,

$p_k := y_k - x_k$ is a feasible descent direction

- ▶ Solve **LP** to find y_k (and p_k), since X polyhedral
- ▶ Search direction towards an extreme point of X
- ▶ This is the basis of the **Frank–Wolfe algorithm**

- ▶ If LP has finite optimum $y_k \implies$ search direction $p_k = y_k - x_k$
- ▶ If LP obj. val. unbounded, simplex method still finds search dir.
- ▶ In this lecture, we assume X bounded for simplicity



Step 0. Find $x_0 \in X$ (e.g. any extreme point in X). Set $k := 0$

Step 1. Find an optimal solution y_k to the problem to

$$\underset{y \in X}{\text{minimize}} \quad z_k(y) := \nabla f(x_k)^T (y - x_k) \quad (2)$$

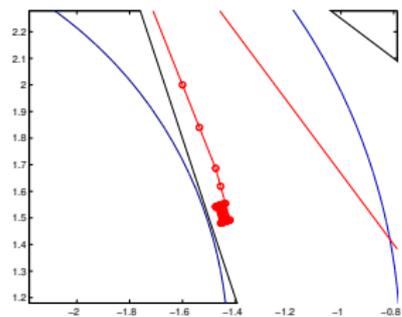
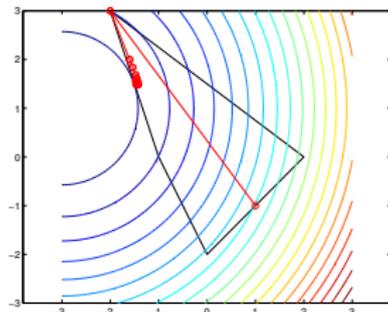
Let $p_k := y_k - x_k$ be the search direction

Step 2. Line search: (approximately) minimize $f(x_k + \alpha p_k)$ over $\alpha \in [0, 1]$. Let α_k be the step length

Step 3. Let $x_{k+1} := x_k + \alpha_k p_k$

Step 4. If, for example, $z_k(y_k)$ or α_k is close to zero, then terminate! Otherwise, let $k := k + 1$ and go to Step 1

- ▶ Suppose $X \subset \mathbb{R}^n$ nonempty **polytope**; f in C^1 on X
- ▶ In Step 2 (line search), we either use an **exact line search** or the **Armijo step length rule**
- ▶ Then: the sequence $\{x_k\}$ is bounded and every limit point (at least one exists) is stationary;
- ▶ If f is convex on X , then every limit point is globally optimal



- ▶ Suppose f is convex on X . Then for each k , $\forall y \in X$ it holds that

$$\begin{aligned} f(y) &\geq f(x_k) + \nabla f(x_k)^T (y - x_k) && \text{(since } f \text{ convex)} \\ &\geq f(x_k) + \nabla f(x_k)^T (y_k - x_k) && \text{(by definition of } y_k) \end{aligned}$$

implying that

$$f^* \geq \underbrace{f(x_k) + \nabla f(x_k)^T (y_k - x_k)}_{\text{lower bound of } f^*}$$

- ▶ Keep the best lower bound (LBD) up to current iteration. That is,

$$\text{LBD} \leftarrow \max \{ \text{LBD}, f(x_k) + \nabla f(x_k)^T (y_k - x_k) \}$$

In step 4, terminate if $f(x_k) - \text{LBD}$ is small enough

- ▶ Frank–Wolfe uses linear approximations—works **best for almost linear problems**
- ▶ For highly nonlinear problems, the approximation is bad—the optimal solution may be far from an extreme point
- ▶ In order to find a near-optimum requires many iterations—the algorithm is **slow**
- ▶ Extreme points in previous iterations forgotten; can speed up by storing and using previous extreme points

- ▶ Representation Theorem (for polytopes):
 - ▶ $P = \{x \in \mathbb{R}^n \mid Ax = b; x \geq 0^n\}$, nonempty and bounded
 - ▶ $V = \{v^1, \dots, v^K\}$ be the set of extreme points of P

Then,

$$x \in P \iff x = \sum_{i=1}^K \alpha_i v^i, \quad \text{for some } \alpha_1, \dots, \alpha_K \geq 0, \quad \sum_{i=1}^K \alpha_i = 1$$

- ▶ **Simplicial decomposition** idea: use some (hopefully few) extreme points to describe optimal solution x^*

$$x^* = \sum_{i \in \mathcal{K}} \alpha_i v^i, \quad |\mathcal{K}| \ll K$$

- ▶ Extreme points of feasible set v^1, \dots, v^K
- ▶ At each iteration k , maintain “working set” $\mathcal{P}_k \subseteq \{v^1, v^2, \dots, v^K\}$
- ▶ Check for stationarity of $x_k \in \mathcal{P}_k$ (just like Frank-Wolfe)
 - ▶ x_k stationary \implies terminate
 - ▶ else, identify (possibly new) extreme pt. y_k ; $\mathcal{P}_{k+1} = \mathcal{P}_k \cup \{y_k\}$
- ▶ Optimize f over $\text{conv}(\mathcal{P}_{k+1} \cup \{x_k\})$ for x_{k+1}
 - restricted master problem, multi-dimensional line search, etc

Step 0. Find $x_0 \in X$, for example any extreme point in X . Set $k := 0$. Let $\mathcal{P}_0 := \emptyset$

Step 1. Let y_k be an optimal solution to the LP problem

$$\underset{y \in X}{\text{minimize}} \quad z_k(y) := \nabla f(x_k)^T (y - x_k)$$

Let $\mathcal{P}_{k+1} := \mathcal{P}_k \cup \{y_k\}$

Step 2. Min f over $\text{conv}(\{x_k\} \cup \mathcal{P}_{k+1})$. Let $(\mu_{k+1}, \nu_{k+1}) \in \mathbb{R} \times \mathbb{R}^{|\mathcal{P}_{k+1}|}$ minimizes *restricted master problem* (RMP)

$$\begin{aligned} \underset{(\mu, \nu)}{\text{minimize}} \quad & f\left(\mu x_k + \sum_{y_i \in \mathcal{P}_{k+1}} \nu(i) y_i\right) \\ \text{subject to} \quad & \mu + \sum_{i=1}^{|\mathcal{P}_{k+1}|} \nu(i) = 1, \\ & \mu, \nu(i) \geq 0, \quad i = 1, 2, \dots, |\mathcal{P}_{k+1}| \end{aligned}$$

Step 3. Let $x_{k+1} := \mu_{k+1} x_k + \sum_{i=1}^{|\mathcal{P}_{k+1}|} \nu_{k+1}(i) y_i$

Step 4. If $z_k(y_k) \approx 0$ or if $\mathcal{P}_{k+1} = \mathcal{P}_k$ then terminate (why?)
Otherwise, let $k := k + 1$ and go to Step 1

- ▶ Basic version keeps adding extreme points: $\mathcal{P}_{k+1} \leftarrow \mathcal{P}_k \cup \{y_k\}$
- ▶ Alternative: drop members of \mathcal{P}_k with small weights in RMP; or set upper bound on $|\mathcal{P}_k|$
- ▶ Special case: $|\mathcal{P}_k| = 1 \implies$ Frank–Wolfe (FW) algorithm!
- ▶ Simplicial decomposition (SD) requires fewer iterations than FW
- ▶ Unfortunately, solving RMP is more difficult than line search
 - ▶ but RMP feasible set structured – unit simplex

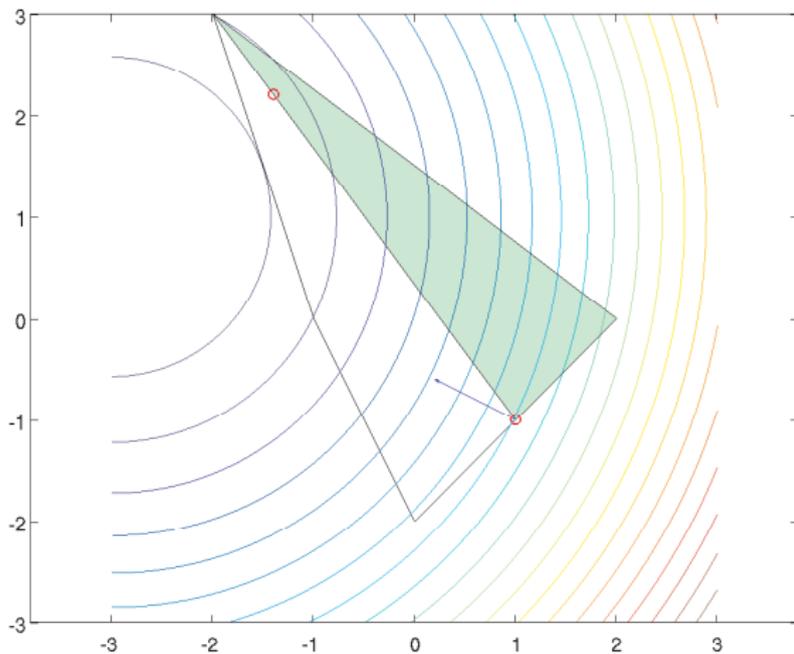


Figure: Example implementation of SD. Starting at $x_0 = (1, -1)^T$, and with \mathcal{P}_0 as the extreme point at $(2, 0)^T$, $|\mathcal{P}_k| \leq 2$.

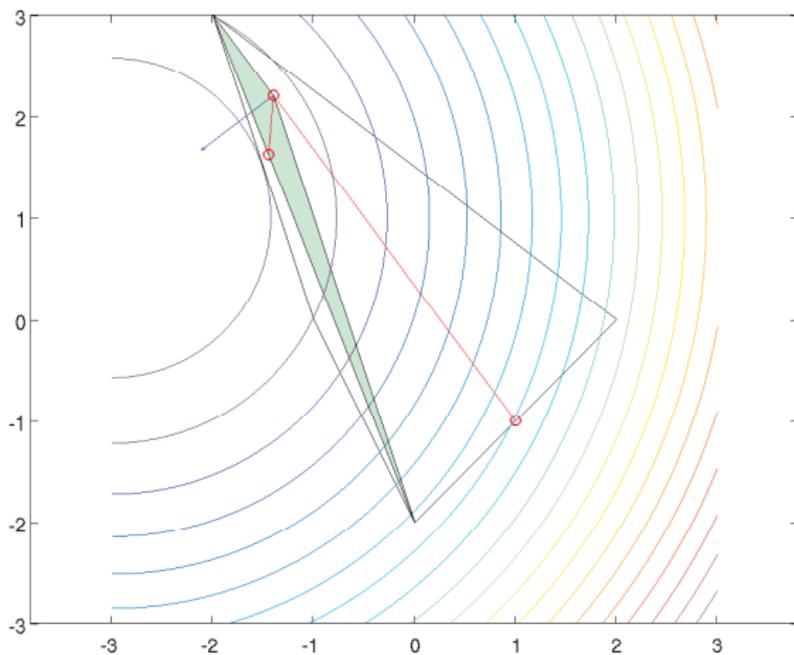


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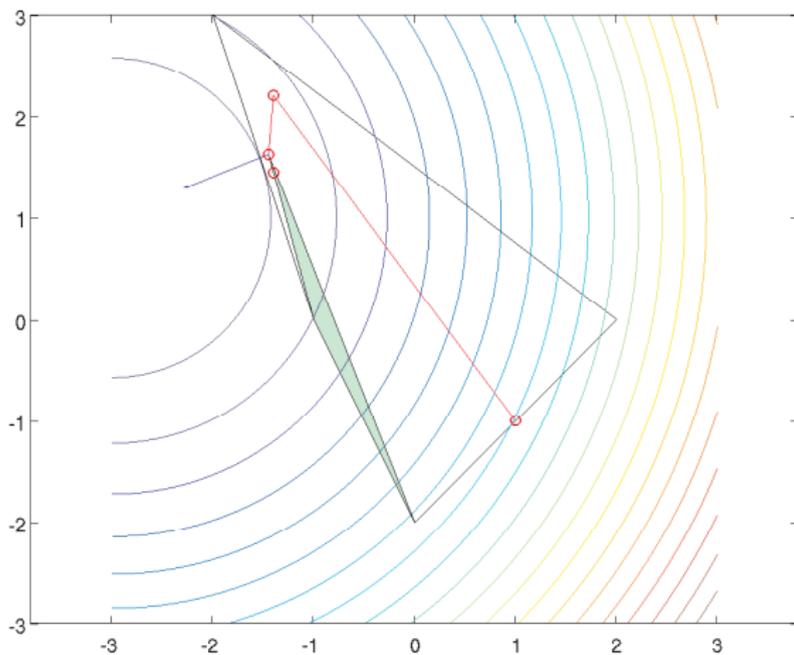


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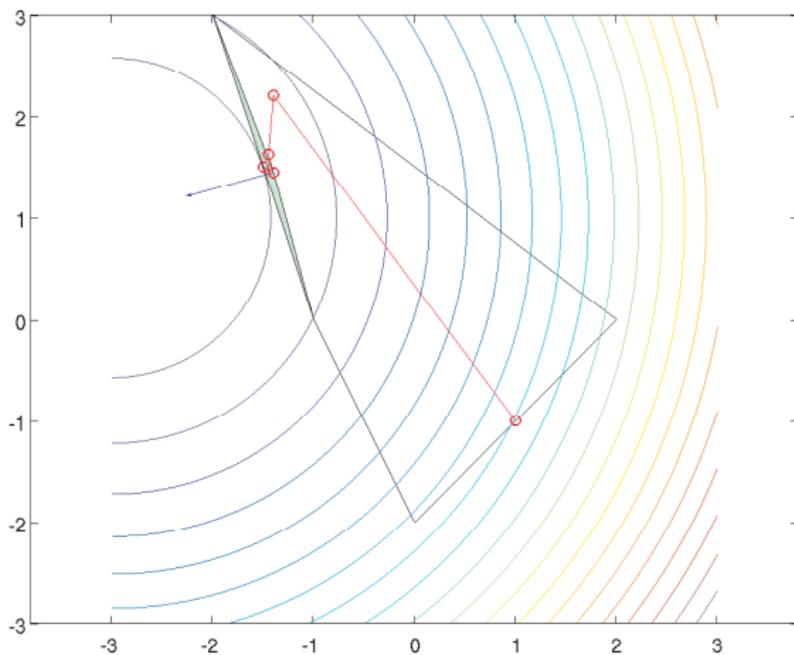


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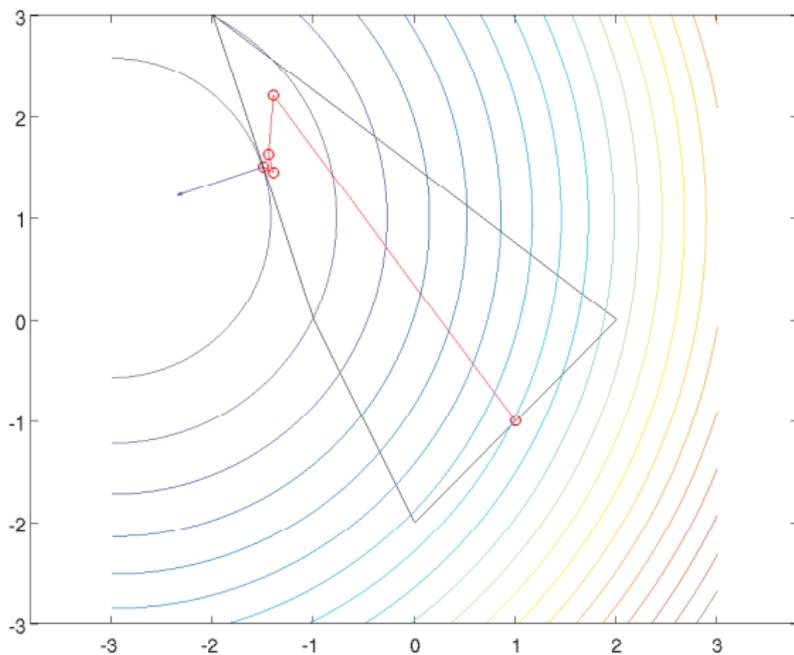
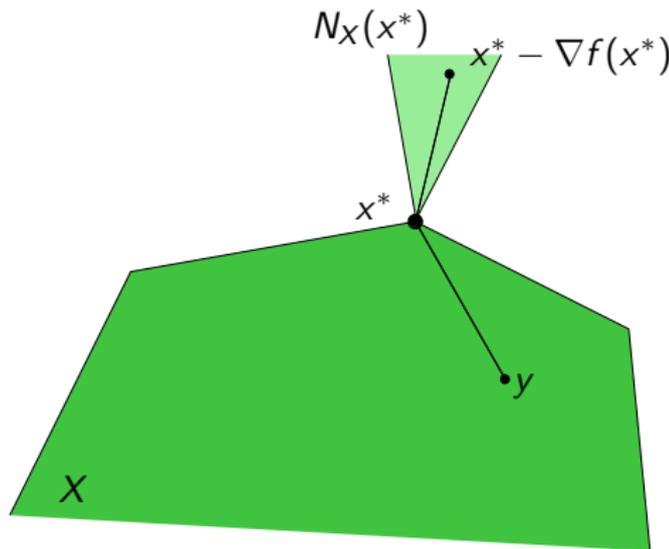


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- ▶ It does at least as well as the Frank–Wolfe algorithm: line segment $[x_k, y_k]$ feasible in RMP
- ▶ SD converges in finite number of iterations if all of following hold
 - ▶ x^* unique
 - ▶ RMP solved exactly
 - ▶ $|\mathcal{P}_k|$ large enough (to represent x^*)
- ▶ Much more efficient than the Frank–Wolfe algorithm in practice (consider example solved by FW and SD)
- ▶ Can solve the RMPs efficiently, since the constraints are simple

- ▶ The gradient projection algorithm based on:

$$x^* \in X \text{ stationary} \iff x^* = \text{Proj}_X[x^* - \alpha \nabla f(x^*)], \quad \forall \alpha > 0$$

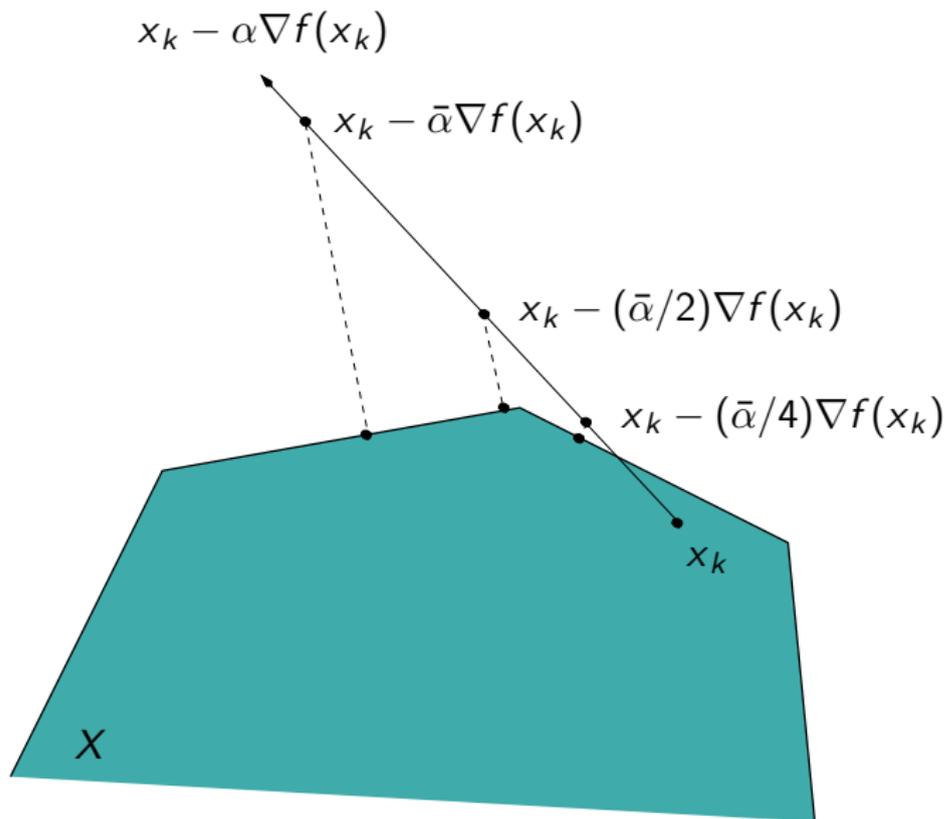


- ▶ x not stationary; $p = \text{Proj}_X[x - \alpha \nabla f(x)] - x \neq 0$ for any $\alpha > 0$
 - ▶ p feasible descent direction
 - ▶ A version of gradient projection method: $x_{k+1} = x_k + \alpha_k p$
- ▶ Another version: gradient projection method with **projection arc**:

$$x_{k+1} := \text{Proj}_X[x_k - \alpha_k \nabla f(x_k)]$$

step size α_k determined using Armijo rule

- ▶ $X = \mathbb{R}^n \implies$ gradient projection becomes steepest descent



- ▶ Bottleneck: how can we compute projections?
- ▶ In general, we study the KKT conditions of the system and apply a simplex-like method.
- ▶ If we have a specially structured feasible polyhedron, projections may be easier to compute.
 - ▶ hypercube $\{x \mid 0 \leq x_i \leq 1, i = 1, \dots, n\}$
 - ▶ unit simplex $\{x \mid \sum_{i=1}^n x_i = 1, x \geq \mathbf{0}\}$ (cf. RMP in simplicial decomposition)

- ▶ Example: the feasible set is $S = \{x \in \mathbb{R}^n \mid 0 \leq x_i \leq 1, i = 1, \dots, n\}$.
- ▶ Then $\text{Proj}_S(x) = z$, where

$$z_i = \begin{cases} 0, & x_i < 0, \\ x_i, & 0 \leq x_i \leq 1 \\ 1, & 1 < x_i, \end{cases}$$

for $i = 1, \dots, n$.

- ▶ Exercise: prove this by applying the variational inequality (or KKT conditions) to the problem

$$\min_{z \in S} \frac{1}{2} \|x - z\|^2$$

- ▶ $X \subseteq \mathbb{R}^n$ nonempty, closed, convex; $f \in C^1$ on X ;
- ▶ for the starting point $x_0 \in X$ it holds that the level set $\text{lev}_f(f(x_0))$ intersected with X is bounded
- ▶ step length α_k is given by the Armijo step length rule along the projection arc
- ▶ Then: the sequence $\{x_k\}$ is bounded;
- ▶ every limit point of $\{x_k\}$ is stationary;
- ▶ $\{f(x_k)\}$ descending, lower bounded, hence convergent
- ▶ Convergence arguments similar to steepest descent one

- ▶ Assume: $X \subseteq \mathbb{R}^n$ nonempty, closed, convex;
- ▶ $f \in C^1$ on X ; f convex;
- ▶ an optimal solution x^* exists
- ▶ In the algorithm (4), the step length α_k is given by the Armijo step length rule along the projection arc
- ▶ Then: the sequence $\{x_k\}$ converges to an optimal solution
- ▶ Note: with $X = \mathbb{R}^n \implies$ convergence of steepest descent for convex problems with optimal solutions!

- ▶ A large-scale nonlinear network flow problem which is used to estimate traffic flows in cities
- ▶ Model over the small city of Sioux Falls in North Dakota, USA; 24 nodes, 76 links, and 528 pairs of origin and destination
- ▶ Three algorithms for the RMPs were tested—a Newton method and two gradient projection methods. MATLAB implementation.
- ▶ Remarkable difference—The Frank–Wolfe method suffers from very small steps being taken. Why? Many extreme points active = many routes used

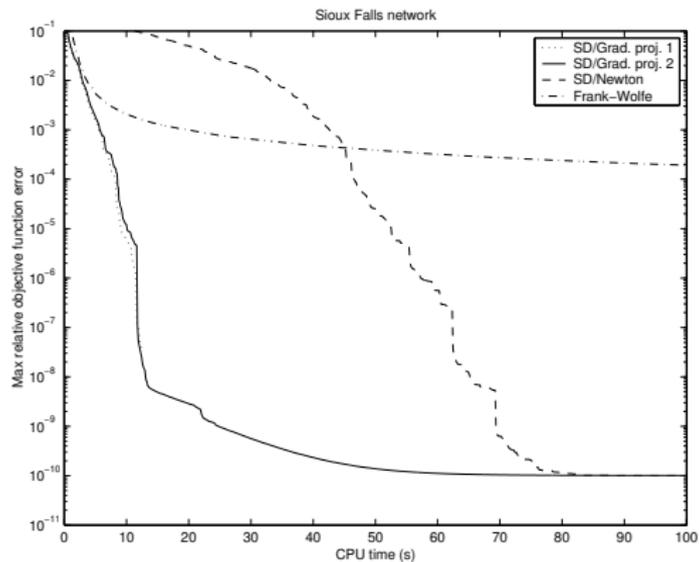


Figure: The performance of SD vs. FW on the Sioux Falls network