Optimisation Combinatoire et Convexe

First Order Methods: Part II

First Order Methods: Part Two.

- Centering. Solve a centering problem at each iteration and compute a subgradient at the center to localize the solution.
- Affine maximization. Solve an affine maximization problem over the feasible set.
- Partial optimization. Solve the minimization problem over a subset of the variables.

Centering: Localization Methods

- Function $f : \mathbb{R}^n \to \mathbb{R}$ convex (and for now, differentiable)
- **problem:** minimize *f*
- oracle model: for any x we can evaluate f and $\nabla f(x)$ (at some cost)

Main assumption: evaluating the gradient is very expensive.

from
$$f(x) \ge f(x_0) + \nabla f(x_0)^T (x - x_0)$$
 we conclude

$$\nabla f(x_0)^T(x-x_0) \ge 0 \implies f(x) \ge f(x_0)$$

i.e., all points in halfspace $\nabla f(x_0)^T(x-x_0) \ge 0$ are **worse** than x_0

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Localization methods



• by evaluating ∇f we rule out a halfspace in our search for x^* :

$$x^{\star} \in \{x \mid \nabla f(x_0)^T (x - x_0) \le 0\}$$

- **idea:** get one bit of info (on location of x^*) by evaluating ∇f
- for nondifferentiable f, can replace $\nabla f(x_0)$ with any subgradient $g \in \partial f(x_0)$

Localization methods

suppose we have evaluated $\nabla f(x_1), \ldots, \nabla f(x_k)$ then we know $x^* \in \{x \mid \nabla f(x_i)^T (x - x_i) \leq 0\}$



on the basis of $\nabla f(x_1), \ldots, \nabla f(x_k)$, we have **localized** x^* to a polyhedron

question: what is a 'good' point x_{k+1} at which to evaluate ∇f ?

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Basic **localization** (or cutting-plane) algorithm:

1. after iteration k-1 we know $x^* \in \mathcal{P}_{k-1}$:

$$\mathcal{P}_{k-1} = \{ x \mid \nabla f(x^{(i)})^T (x - x^{(i)}) \le 0, \ i = 1, \dots, k-1 \}$$

2. evaluate $\nabla f(x^{(k)})$ (or $g \in \partial f(x^{(k)})$) for some $x^{(k)} \in \mathcal{P}_{k-1}$

3.
$$\mathcal{P}_k := \mathcal{P}_{k-1} \cap \{ x \mid \nabla f(x^{(k)})^T (x - x^{(k)}) \le 0 \}$$

Localization methods



- \mathcal{P}_k gives our uncertainty of x^\star at iteration k
- want to pick $x^{(k)}$ so that \mathcal{P}_{k+1} is as small as possible
- clearly want $x^{(k)}$ near center of $C^{(k)}$

Example: bisection on \mathbb{R}

- $\bullet f: \mathbb{R} \to \mathbb{R}$
- \mathcal{P}_k is interval
- obvious choice: $x^{(k+1)} := \operatorname{midpoint}(\mathcal{P}_k)$

bisection algorithm

given interval C = [l, u] containing x^*

repeat

- 1. x := (l+u)/2
- 2. evaluate f'(x)
- 3. if f'(x) < 0, l := x; else u := x

Example: bisection on $\mathbb R$



$$\mathsf{length}(\mathcal{P}_{k+1}) = u_{k+1} - l_{k+1} = \frac{u_k - l_k}{2} = (1/2)\mathsf{length}(\mathcal{P}_k)$$

and so $\text{length}(\mathcal{P}_k) = 2^{-k} \text{length}(\mathcal{P}_0)$

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interpretation:

- length(\mathcal{P}_k) measures our uncertainty in x^{\star}
- uncertainty is halved at each iteration; get exactly one bit of info about x^{\star} per iteration
- # steps required for uncertainty (in x^*) $\leq \epsilon$:

$$\log_2 \frac{\text{length}(\mathcal{P}_0)}{\epsilon} = \log_2 \frac{\text{initial uncertainty}}{\text{final uncertainty}}$$

question:

- can bisection be extended to \mathbb{R}^n ?
- or is it special since \mathbb{R} is linear ordering?

Center of gravity algorithm

Take $x^{(k+1)} = CG(\mathcal{P}_k)$ (center of gravity)

$$\mathsf{CG}(\mathcal{P}_k) = \int_{\mathcal{P}_k} x \, dx \, \bigg/ \int_{\mathcal{P}_k} dx$$

theorem. if $C \subseteq \mathbb{R}^n$ convex, $x_{cg} = CG(C)$, $g \neq 0$,

$$\operatorname{vol}(C \cap \{x \mid g^T(x - x_{cg}) \le 0\}) \le (1 - 1/e) \operatorname{vol}(C) \approx 0.63 \operatorname{vol}(C)$$

(independent of dimension n)

hence in CG algorithm, $\mathbf{vol}(\mathcal{P}_k) \leq 0.63^k \mathbf{vol}(\mathcal{P}_0)$

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- $\mathbf{vol}(\mathcal{P}_k)^{1/n}$ measures uncertainty (in x^*) at iteration k
- uncertainty reduced at least by $0.63^{1/n}$ each iteration
- from this can prove $f(x^{(k)}) \to f(x^{\star})$ (later)
- **•** max. # steps required for uncertainty $\leq \epsilon$:

$$1.51n \log_2 \frac{\text{initial uncertainty}}{\text{final uncertainty}}$$

(cf. bisection on \mathbb{R})

advantages of CG-method

- guaranteed convergence
- number of steps proportional to dimension n, log of uncertainty reduction

disadvantages

- finding $x^{(k+1)} = CG(\mathcal{P}_k)$ is **harder** than original problem
- \mathcal{P}_k becomes more complex as k increases (removing redundant constraints is harder than solving original problem)

(but, can modify CG-method to work)

analytic center of polyhedron $\mathcal{P} = \{z \mid a_i^T z \leq b_i, i = 1, \dots, m\}$ is

$$\mathsf{AC}(\mathcal{P}) = \underset{z}{\operatorname{argmin}} - \sum_{i=1}^{m} \log(b_i - a_i^T z)$$

ACCPM is localization method with next query point $x^{(k+1)} = AC(\mathcal{P}_k)$ (found by Newton's method)

• let x^* be analytic center of $\mathcal{P} = \{z \mid a_i^T z \leq b_i, i = 1, \dots, m\}$

• let H^* be Hessian of barrier at x^* ,

$$H^* = -\nabla^2 \sum_{i=1}^m \log(b_i - a_i^T z) \bigg|_{z=x^*} = \sum_{i=1}^m \frac{a_i a_i^T}{(b_i - a_i^T x^*)^2}$$

• then, $\mathcal{P} \subseteq \mathcal{E} = \{ z \mid (z - x^*)^T H^*(z - x^*) \leq m^2 \}$ (not hard to show)

- \blacksquare let $\mathcal{E}^{(k)}$ be outer ellipsoid associated with $x^{(k)}$
- \blacksquare a lower bound on optimal value p^{\star} is

$$p^{\star} \geq \inf_{z \in \mathcal{E}^{(k)}} \left(f(x^{(k)}) + g^{(k)T}(z - x^{(k)}) \right)$$
$$= f(x^{(k)}) - m_k \sqrt{g^{(k)T} H^{(k)-1} g^{(k)}}$$

 $(m_k \text{ is number of inequalities in } \mathcal{P}_k)$

• gives simple stopping criterion $\sqrt{g^{(k)T}H^{(k)-1}g^{(k)}} \leq \epsilon/m_k$

Best objective and lower bound

since ACCPM isn't a descent a method, we keep track of best point found, and best lower bound

best function value so far: $u_k = \min_{i=1,...,k} f(x^{(k)})$

best lower bound so far: $l_k = \max_{i=1,...,k} f(x^{(k)}) - m_k \sqrt{g^{(k)T} H^{(k)-1} g^{(k)}}$

can stop when $u_k - l_k \leq \epsilon$

given polyhedron \mathcal{P} containing x^* repeat 1. compute x^* , the analytic center of \mathcal{P} , and H^* 2. compute $f(x^*)$ and $g \in \partial f(x^*)$ 3. $u := \min\{u, f(x^*)\}$ $l := \max\{l, f(x^*) - m\sqrt{g^T H^{*-1}g}\}$ 4. add inequality $g^T(z - x^*) \leq 0$ to \mathcal{P} until $u - l < \epsilon$

here m is number of inequalities in \mathcal{P}

ACCPM adds an inequality to ${\cal P}$ each iteration, so centering gets harder, more storage as algorithm progresses

schemes for **dropping constraints** from $\mathcal{P}^{(k)}$:

- remove all redundant constraints (expensive)
- remove some constraints known to be redundant
- remove constraints based on some relevance ranking

 x^* is AC of $\mathcal{P} = \{x \mid a_i^T x \leq b_i, i = 1, \dots, m\}$, H^* is barrier Hessian at x^*

define (ir)relevance measure
$$\eta_i = \frac{b_i - a_i^T x^*}{\sqrt{a_i^T H^{*-1} a_i}}$$

• η_i/m is normalized distance from hyperplane $a_i^T x = b_i$ to outer ellipsoid

• if $\eta_i \ge m$, then constraint $a_i^T x \le b_i$ is redundant

common ACCPM constraint dropping schemes:

- drop all constraints with $\eta_i \geq m$ (guaranteed to not change \mathcal{P})
- drop constraints in order of irrelevance, keeping constant number, usually 3n 5n

Example

PWL objective, n = 10 variables, m = 100 terms

simple ACCPM: $f(x^{(k)})$ and lower bound $f(x^{(k)}) - m\sqrt{g^{(k)T}H^{(k)-1}g^{(k)}}$



ACCPM with constraint dropping



ACCPM with constraint dropping

number of inequalities in \mathcal{P} :



... constraint dropping actually **improves** convergence (!)

Challenges in cutting-plane methods:

- can be difficult to compute appropriate next query point
- Iocalization polyhedron grows in complexity as algorithm progresses

can get around these challenges . . .

ellipsoid method is another approach

- developed in 70s by Shor and Yudin
- used in 1979 by Khachian to give polynomial time algorithm for LP

idea: localize x^{\star} in an ellipsoid instead of a polyhedron

- 1. at iteration k we know $x^{\star} \in \mathcal{E}^{(k)}$
- 2. set $x^{(k+1)} := \operatorname{center}(\mathcal{E}^{(k)})$; evaluate $\nabla f(x^{(k+1)})$ (or $g^{(k)} \in \partial f(x^{(k+1)})$)
- 3. hence we know

$$x^{\star} \in \mathcal{E}^{(k)} \cap \{ z \mid \nabla f(x^{(k+1)})^T (z - x^{(k+1)}) \le 0 \}$$

(a half-ellipsoid)

4. set $\mathcal{E}^{(k+1)} :=$ minimum volume ellipsoid covering $\mathcal{E}^{(k)} \cap \{z \mid \nabla f(x^{(k+1)})^T (z - x^{(k+1)}) \leq 0\}$

Ellipsoid algorithm



compared to cutting-plane method:

- Iocalization set doesn't grow more complicated
- easy to compute query point
- but, we add unnecessary points in step 4

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- $\hfill\blacksquare$ reduces to bisection for n=1
- simple formula for $\mathcal{E}^{(k+1)}$ given $\mathcal{E}^{(k)}$, $\nabla f(x^{(k+1)})$
- $\mathcal{E}^{(k+1)}$ can be larger than $\mathcal{E}^{(k)}$ in diameter (max semi-axis length), but is always smaller in volume
- $\operatorname{vol}(\mathcal{E}^{(k+1)}) < e^{-\frac{1}{2n}} \operatorname{vol}(\mathcal{E}^{(k)})$

(note that volume reduction factor depends on n)

Example



Updating the ellipsoid

$$\mathcal{E}(x,A) = \left\{ z \mid (z-x)^T A^{-1} (z-x) \le 1 \right\}$$



(for n > 1) minimum volume ellipsoid containing

$$\mathcal{E} \cap \left\{ z \mid g^T(z-x) \le 0 \right\}$$

is given by

$$x^{+} = x - \frac{1}{n+1} A \tilde{g}$$
$$A^{+} = \frac{n^{2}}{n^{2} - 1} \left(A - \frac{2}{n+1} A \tilde{g} \tilde{g}^{T} A \right)$$

where $\tilde{g} \stackrel{\Delta}{=} g \left/ \sqrt{g^T A g} \right|$

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As in the ACCPM case, we can get **error bounds** on the current iterate.

 $x^\star \in \mathcal{E}_k$, so

$$f(x^{\star}) \geq f(x^{(k)}) + \nabla f(x^{(k)})^T (x^{\star} - x^{(k)})$$

$$\geq f(x^{(k)}) + \inf_{x \in \mathcal{E}^{(k)}} \nabla f(x^{(k)})^T (x - x^{(k)})$$

$$= f(x^{(k)}) - \sqrt{\nabla f(x^{(k)})^T A^{(k)} \nabla f(x^{(k)})}$$

simple stopping criterion:

$$\sqrt{\nabla f(x^{(k)})^T A^{(k)} \nabla f(x^{(k)})} \le \epsilon$$

Stopping criterion



Basic ellipsoid algorithm

ellipsoid described as $\mathcal{E}(x, A) = \{ z \mid (z - x)^T A^{-1} (z - x) \leq 1 \}$

given ellipsoid $\mathcal{E}(x, A)$ containing x^* , accuracy $\epsilon > 0$ repeat

1. evaluate $\nabla f(x)$ (or $g \in \partial f(x)$) 2. if $\sqrt{\nabla f(x)^T A \nabla f(x)} \leq \epsilon$, return(x) 3. update ellipsoid 3a. $\tilde{g} := \nabla f(x) / \sqrt{\nabla f(x)^T A \nabla f(x)}$ 3b. $x := x - \frac{1}{n+1} A \tilde{g}$ 3c. $A := \frac{n^2}{n^2 - 1} \left(A - \frac{2}{n+1} A \tilde{g} \tilde{g}^T A \right)$

properties:

- can propagate Cholesky factor of A; get $O(n^2)$ update
- not a descent method
- often slow but robust in practice

- change coordinates so uncertainty (\mathcal{E}) is unit ball
- take gradient (or subgradient) step with fixed length 1/(n+1)

properties:

- can propagate Cholesky factor of A; get $O(n^2)$ update
- **not** a descent method
- often slow but robust in practice

Proof of convergence

assumptions:

• f is Lipschitz: $|f(y) - f(x)| \le G ||y - x||$ • $\mathcal{E}^{(0)}$ is ball with radius R

suppose $f(x^{(i)}) > f^{\star} + \epsilon$, $i = 0, \dots, k$, then

$$f(x) \le f^\star + \epsilon \Longrightarrow x \in \mathcal{E}^{(k)}$$

since at iteration i we only discard points with $f \ge f(x^{(i)})$, then from Lipschitz condition,

$$||x - x^{\star}|| \le \epsilon/G \Longrightarrow f(x) \le f^{\star} + \epsilon \Longrightarrow x \in \mathcal{E}^{(k)}$$

so $B = \{x \mid ||x - x^*|| \le \epsilon/G\} \subseteq \mathcal{E}^{(k)}$, hence $\operatorname{vol}(B) \le \operatorname{vol}(\mathcal{E}^{(k)})$, so

$$\beta_n(\epsilon/G)^n \le e^{-k/2n} \operatorname{vol}(\mathcal{E}^{(0)}) = e^{-k/2n} \beta_n R^n$$

 $(\beta_n \text{ is volume of unit ball in } \mathbb{R}^n)$, therefore $k \leq 2n^2 \log(RG/\epsilon)$

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conclusion: for $K > 2n^2 \log(RG/\epsilon)$,

$$\min_{i=0,\dots,K} f(x^{(i)}) \le f^* + \epsilon$$

since $x^* \in \mathcal{E}_0 = \{x \mid ||x - x^{(0)}|| \le R\}$, our prior knowledge of f^* is $f^* \in [f(x^{(0)}) - GR, f(x^{(0)})]$

our prior uncertainty in f^{\star} is GR

after k iterations our knowledge of f^\star is

$$f^{\star} \in \left[\min_{i=0,...,k} f(x^{(i)}) - \epsilon, \min_{i=0,...,k} f(x^{(i)})\right]$$

posterior uncertainty in f^* is $\leq \epsilon$

iterations required:

$$2n^2 \log \frac{RG}{\epsilon} = 2n^2 \log \frac{\text{prior uncertainty}}{\text{posterior uncertainty}}$$

efficiency: $0.72/n^2$ bits per gradient evaluation (degrades with n)

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$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \ i=1,\ldots,m \end{array}$$

same idea: maintain ellipsoids $\mathcal{E}^{(k)}$ that

- \blacksquare contain x^\star
- decrease in volume to zero

case 1: $x^{(k)}$ feasible, *i.e.*, $f_i(x^{(k)}) \le 0$, i = 1, ..., m

- then do usual update of $\mathcal{E}^{(k)}$ based on $abla f_0(x^{(k)})$
- rules out halfspace of points with larger function value than current point

case 2:
$$x^{(k)}$$
 infeasible, say, $f_j(x^{(k)}) > 0$;

- then $\nabla f_j(x^{(k)})^T(x-x^{(k)}) \ge 0 \Longrightarrow f_j(x) > 0 \Longrightarrow x$ infeasible so update $\mathcal{E}^{(k)}$ based on $\nabla f_j(x^{(k)})$
- rules out halfspace of infeasible points

Affine Maximization: Frank-Wolfe

Classical first order methods for solving

 $\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in C, \end{array}$

in $x \in \mathbb{R}^n$, with $C \subset \mathbb{R}^n$ convex, relied on the assumption that the following subproblem could be solved efficiently

 $\begin{array}{ll} \mbox{minimize} & y^T x + d(x) \\ \mbox{subject to} & x \in C, \end{array}$

in the variable $x \in \mathbb{R}^n$, where d(x) is a strongly convex function.

The method detailed here assumes instead that the affine minimization subproblem

minimize $d^T x$ subject to $x \in C$

can be solved efficiently for any $y \in \mathbb{R}^n$.

Algorithm.

• Choose $x_0 \in C$.

• For $k = 1, \ldots, k^{max}$ iterate

- 1. Compute $\nabla f(x_k)$
- 2. Solve

minimize $x^T \nabla f(y_k)$ subject to $x \in C$

in $x \in \mathbb{R}^n$, call the solution x_d .

3. Update the current point

$$x_{k+1} = x_k + \frac{2}{k+2}(x_d - x_k)$$

Note that all iterates are feasible.

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Complexity. Assume that f is differentiable. Define the curvature C_f of the function f(x) as

$$C_f \triangleq \sup_{\substack{s,x \in \mathcal{M}, \ \alpha \in [0,1], \\ y=x+\alpha(s-x)}} \frac{1}{\alpha^2} (f(y) - f(x) - \langle y - x, \nabla f(x) \rangle).$$

The Franke-Wolfe algorithm will then produce an ϵ solution after

$$N_{\max} = \frac{4C_f}{\epsilon}$$

iterations.

Stopping criterion. At each iteration, we get a lower bound on the optimum as a byproduct of the affine minimization step. By convexity

$$f(x_k) + \nabla f(x_k)^T (x_d - x_k) \le f(x), \text{ for all } x \in C$$

and finally, calling f^* the optimal value of problem, we obtain

$$f(x_k) - f^* \le \nabla f(x_k)^T (x_k - x_d).$$

This allows us to bound the suboptimality of iterate at no additional cost.

Partial Minimization: Coordinate Descent

We seek to solve

 $\begin{array}{ll} \mbox{minimize} & f(x) \\ \mbox{subject to} & x \in C \end{array}$

in the variable $x \in \mathbb{R}^n$, with $C \subset \mathbb{R}^n$ convex.

Our main assumption here is that C is a product of simpler sets. We rewrite the problem

 $\begin{array}{ll} \text{minimize} & f(x_1,\ldots,x_p) \\ \text{subject to} & x_i \in C_i, \quad i=1,\ldots,p \end{array}$

where $C = C_1 \times \ldots \times C_p$.

This helps if the minimization subproblems

$$\min_{x_i \in C_i} f(x_1, \dots, x_i, \dots, x_p)$$

can be solved very efficiently (or in closed-form).

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Algorithm. The algorithm simply computes the iterates $x^{(k+1)}$ as

$$x_{i}^{(k+1)} = \operatorname{argmin}_{x_{i} \in C_{i}} f(x_{1}^{(k)}, \dots, x_{i}^{(k)}, \dots, x_{p}^{(k)})$$
$$x_{j}^{(k+1)} = x_{j}^{(k)}, \quad j \neq i$$

for a certain $i \in [1, p]$, cycling over all indices in [1, p].

Convergence.

- Complexity analysis similar to coordinate-wise gradient descent (or steepest descent in ℓ_1 norm).
- Need f(x) strongly convex to get linear complexity bound.
- Few clean results outside of this setting.

Example.

Consider the box constrained minimization problem

 $\begin{array}{ll} \mbox{minimize} & x^TAx + b^Tx\\ \mbox{subject to} & \|x\|_\infty \leq 1 \end{array}$

in the variable $x \in \mathbb{R}^n$. We assume $A \succ 0$.

- The set $||x||_{\infty} \leq 1$ is a box, i.e. a product of intervals.
- Each minimization subproblem means solving a second order equation.
- The dual is

$$\min_{y \in \mathbb{R}^n} (b+y)^T A^{-1}(b+y) - 4 \|y\|_1$$

which can be interpreted as a penalized regression problem in the variable $y \in \mathbb{R}^n$.

Partial Minimization:

Dykstra, alternating projection

We focus on a simple feasibility problem

find $x \in C_1 \cap C_2$

in the variable $x \in \mathbb{R}^n$ with $C_1, C_2 \subset \mathbb{R}^n$ two convex sets.

We assume now that the projection problems on C_i are easier to solve

minimize $||x - y||_2$ subject to $x \in C_i$

in $x \in \mathbb{R}^n$.

Dykstra, alternating projection

Algorithm (alternating projection)

- Choose $x_0 \in \mathbb{R}^n$.
- For $k = 1, \ldots, k^{max}$ iterate
 - 1. Project on C_1

$$x_{k+1/2} = \underset{x \in C_1}{\operatorname{argmin}} \|x - x_k\|_2$$

2. Project on C_2

$$x_{k+1} = \operatorname*{argmin}_{x \in C_2} \|x - x_{k+1/2}\|_2$$

Convergence. We can show $\operatorname{dist}(x_k, C_1 \cap C_2) \to 0$. Linear convergence provided some additional regularity assumptions.

Algorithm (Dykstra)

- Choose $x_0, z_0 \in \mathbb{R}^n$.
- For $k = 1, \ldots, k^{max}$ iterate
 - 1. Project on C_1

$$x_{k+1/2} = \operatorname*{argmin}_{x \in C_1} \|x - z_k\|_2$$

2. Update

$$z_{k+1/2} = 2x_{k+1/2} - z_k$$

3. Project on C_2

$$x_{k+1} = \operatorname*{argmin}_{x \in C_2} \|x - z_{k+1/2}\|_2$$

4. Update

$$z_{k+1} = z_k + x_{k+1} - x_{k+1/2}$$

Convergence. Usually faster than simple alternating projection.