A practical dual gradient-projection method for large-scale, strictly-convex quadratic programming

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STFC Rutherford Appleton Laboratory

with

Jonathan Hogg & Jennifer Scott

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \frac{1}{2} x^T H x + g^T x \quad \text{subject to} \quad Ax \geq b$$

Manchester-NAG-RAL Workshop
The University of Manchester, 23rd October 2013

Summary of the talk

- optimization at RAL
- convex quadratic programming
- bound-constrained QP via gradient projection
- duality
- dual gradient-projection methods for QP
- DQP
- conclusions

Optimization at RAL

- V chapter in Harwell Subroutine Library (later HSL)
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- GALAHAD library in 2003 replaces V chapter (G., Orban, Toint)
  - CUTEr in 2004, CUTEst in 2013 (G., Orban, Toint)

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- various support (root finding, scaling, presolving, preconditioning . . .)

Linear algebraic needs

Sparse linear equations $Ax = b$

- usually symmetric, often indefinite, sometimes block structured
- good preconditioners for generic and PDE-constrained problems
- singular systems and Fredholm alternatives
- sparse right-hand sides
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Traditionally strong RAL group interactions on subjects such as these

Today's problem: quadratic programming

$$\textbf{QP:} \quad \underset{x \in \mathbb{R}^n}{\text{minimize}} \; q(x) = \tfrac{1}{2} x^T H x + g^T x \;\; \text{subject to} \;\; Ax \geq b$$

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- aim to satisfy (KKT) **criticality conditions**

$$\begin{aligned} Ax_* &\geq b && \text{(primal feasibility)} \\ g + Hx_* - A^T y_* = 0 \;\&\; y_* &\geq 0 && \text{(dual feasibility)} \\ (Ax_* - b) \cdot y_* &= 0 && \text{(complementary slackness)} \end{aligned}$$

or to deduce that the problem is infeasible

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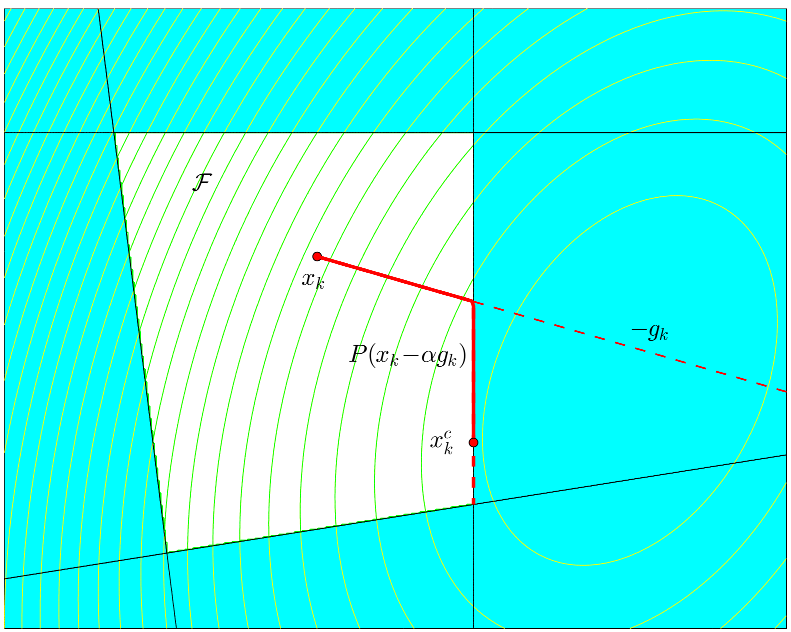
- easy extension to more general constraint structures (equations, upper and both-sided bounds, simple bounds, ...)
- many real-world applications as well as SQP

Competing methods

- interior-point methods
  - usually very efficient
  - relatively poor at warm starting
- active-set methods
  - worst-case combinatorics due to pedestrian active-set changes
  - good at warm starting
- gradient projection methods
  - more rapid active-set changes
  - restricted to constraint sets for which projection is “easy”

Digression I: gradient projection

- convergence and active-set determination driven by projection
  - current iterate $x_k \in \mathcal{F} = \{x : Ax \geq b\}$
  - current gradient $g_k = Hx_k + g$
  - improved **Cauchy point** $x_k^c = P[x_k - \alpha_k g_k]$
  - projection $P[y] = \arg\min_{x \in \mathcal{F}} \|y - x\|$
  - step length $\alpha_k \approx \arg\min q(P[x_k - \alpha g_k])$ (Rosen,1960)



Accelerated gradient projection

- acceleration by subspace minimization
  - pick active set as subset of constraints $\mathcal{A}_k$ active at x_k^c
  - find (approximate) solution s_k to **equality constrained** QP

$$\textbf{EQP:} \quad \underset{s \in \mathbb{R}^n}{\text{minimize}} \;\; q(x_k^c + s) \;\; \text{subject to} \;\; A_{\mathcal{A}_k} s = 0$$

  - set $x_{k+1} \approx \arg\min q(P[x_k^c + \alpha s_k])$

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  - direct factorization (HSL, PARDISO, WSMP,...)

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  - factorization-free projected CG (G., Hribar & Nocedal, Luksan & Vlcek,90s...)

Projected search within simple bounds $x^L \leq x \leq x^U$

Find $\alpha^+ \approx \arg\min q(P[x + \alpha s])$ for $\alpha \geq 0$ (Conn, G. & Toint,1988)

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- approximate "Armijo"projected search also possible (Moré & Toraldo,Toint,90s)

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Anecdotal and empirical evidence

- large change possible in the active set per iteration
- often very effective in practice for convex bound-constrained QP
  - few overall iterations compared to active-set methods (Moré & Toraldo)
  - competitive with interior-point methods for such problems
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How might we apply such methods for QP over a general polyhedral feasible region?

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$$g^T x = y^T Ax - x^T Hx = y^T (s + b) - x^T Hx \geq y^T b - x^T Hx$$

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Suppose $g = A^T y - Hx, \ Ax = s + b$ and $(s, y) \geq 0 \implies$

$$g^T x = y^T Ax - x^T Hx = y^T(s + b) - x^T Hx \geq y^T b - x^T Hx$$

$$\implies q(x) \geq -\tfrac{1}{2}x^T Hx + b^T y$$

Digression II: duality

$$\textbf{QP}: \quad \underset{x}{\text{minimize}} \quad q(x) = \tfrac{1}{2}x^T Hx + g^T x \text{ subject to } Ax \geq b$$

$$\Longleftrightarrow \quad \underset{x,s}{\text{minimize}} \; q(x) \text{ subject to } Ax - s = b \text{ and } s \geq 0 \Longrightarrow (\textbf{KKT})$$

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Suppose $g = A^T y - Hx, \;\; Ax = s + b$ and $(s, y) \geq 0 \Longrightarrow$

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$\Longrightarrow \; q(x) \geq -\tfrac{1}{2}x^T Hx + b^T y \;\; \Longrightarrow$ equivalent **dual problem**

$$\textbf{DQP}: \quad \underset{x,y}{\text{maximize}} \; -\tfrac{1}{2}x^T Hx + b^T y \text{ s.t. } Hx - A^T y = -g \;\&\; y \geq 0$$

Duality II

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$\Longleftrightarrow$ (nonsingular H)

$$\textbf{DQP}: \quad \underset{y}{\text{minimize}} \; \tfrac{1}{2}(y^T A - g^T)H^{-1}(A^T y - g) - b^T y \text{ s.t. } y \geq 0$$

Dual gradient projection methods

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- for strictly-convex QP (i.e., H positive definite)
- dual objective $q_{\rm D}(y) = \frac{1}{2} y^T H_{\rm D} y + g_{\rm D}^T y$
  - $H_{\rm D} = A H^{-1} A^T$ and $g_{\rm D} = -A H^{-1} g - b$
- $H_{\rm D}$ may only be positive semi-definite
- since feasible region is simple, can use gradient projection to allow rapid changes in active set
- require **sparse factorization** $H = LL^T$ but everything else "matrix-free"

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Questions:

- can we perform projected search efficiently?
- can we perform subspace minimization efficiently?

Dual projected search

- have $H_{\mathrm{D}} = AH^{-1}A^T$ and $g_{\mathrm{D}} = -AH^{-1}g - b$
- recall require $\alpha^+ \approx \arg\min q_{\mathrm{D}}(P[y + \alpha s])$ for $\alpha \geq 0$
- investigate for $\alpha = \alpha_i + \Delta\alpha \leq \alpha_{i+1}$ and $y_i = P[y_i + \alpha_i s]$:
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- recur via $H_{\mathrm{D}} s_i = H_{\mathrm{D}} s_{i-1} - H_{\mathrm{D}} \Delta s_i$ with very sparse Δs_i but likely **dense** H_{D} …looks expensive ☹

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- required $y_i^T H_{\mathrm{D}} s_i \equiv u_i^T v_i$ looks harder as update to v_i is dense … but can also be performed using inner-products involving Δu_i
- sparse forward solves now available for HSL solvers `HSL_MA57/87/97` ☺

Dual subspace minimization

- acceleration by subspace minimization along $\boldsymbol{y}_k^c + \boldsymbol{s}$
  - partition variables $\boldsymbol{s}$ into active $\boldsymbol{s}_{\mathrm{A}_k}$ and free $\boldsymbol{s}_{\mathrm{F}_k}$ components according to status of $\boldsymbol{y}_k^c$
  - find (approximate) solution $\boldsymbol{s}_k$ to

$$\text{EQP}: \quad \underset{\boldsymbol{s} \in \mathbb{R}^m}{\text{minimize}} \quad q_{\mathrm{D}}(\boldsymbol{y}_k^c + \boldsymbol{s}) \quad \text{subject to} \quad \boldsymbol{s}_{\mathrm{A}_k} = \boldsymbol{0}$$

  - set $\boldsymbol{y}_{k+1} \approx \arg\min q_{\mathrm{D}}(\boldsymbol{P}[\boldsymbol{y}_k^c + \alpha \boldsymbol{s}_k])$

Dual subspace minimization

- acceleration by subspace minimization along $y_k^c + s$
  - partition variables s into active s_{A_k} and free s_{F_k} components according to status of y_k^c
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$$\text{EQP}: \quad \underset{s \in \mathbb{R}^m}{\text{minimize}} \quad q_{\mathrm{D}}(y_k^c + s) \quad \text{subject to} \quad s_{\mathrm{A}_k} = 0$$

  - set $y_{k+1} \approx \arg\min q_{\mathrm{D}}(P[y_k^c + \alpha s_k])$
- EQP equivalent to $\underset{s \in \mathbb{R}^{m_k}}{\text{minimize}} \quad \frac{1}{2} s^T H_k s + g_k^T s$
  - $H_k = A_k H^{-1} A_k^T$ and $g_k = -A_k H^{-1}(g - A_k^T y_k^c) - b_k$
  - A_k and b_k are respectively the rows of A and components of b corresponding to the m_k free components s_{F_k}
  - H_k is positive semi-definite but may be singular

Digression III: the Fredholm Alternative

$$\textbf{DEQP}: \quad \underset{s \in \mathbb{R}^{m_k}}{\text{minimize}} \quad q_k(s) = \tfrac{1}{2} s^T H_k s + g_k^T s$$

Two possibilities:

1. q_k has a finite critical point s_k for which

$$H_k s_k = -g_k$$

- always if H_k is positive definite
- true if $g_k \in \text{Range}(H_k)$

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2. q_k decreases linearly without bound along a direction s_k for which

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This is the **Fredholm Alternative** for the data $[H_k, g_k]$

The structured Fredholm Alternative

Seek Fredholm Alternative for data $[H_k, g_k]$ where

$$H_k = A_k H^{-1} A_k^T \text{ and } g_k = A_k H^{-1}(A_k^T y_k^c - g) - b_k$$

- $H_k s_k = -g_k$ equivalent to

$$\begin{pmatrix} H & A_k^T \\ A_k & 0 \end{pmatrix} \begin{pmatrix} t_k \\ -s_k \end{pmatrix} = \begin{pmatrix} A_k^T y_k^c - g \\ b_k \end{pmatrix}$$

  for auxiliary unknowns t_k

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$$\left[\begin{pmatrix} H & A_k^T \\ A_k & 0 \end{pmatrix}, \begin{pmatrix} A_k^T y_k^c - g \\ b_k \end{pmatrix} \right]$$

  gives required alternative $H_k s_k = 0$ and $g_k^T s_k < 0$
  $\iff$ $[H_k, g_k]$ is inconsistent

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- HSL sparse solvers `HSL_MA57/86/97` now provide Fredholm Alternative

Alternative to the Fredholm Alternative

$$\textbf{DEQP}: \quad \underset{s \in \mathbb{R}^{m_k}}{\text{minimize}} \quad q_k(s) = \tfrac{1}{2} s^T H_k s + g_k^T s$$

$$H_k = A_k H^{-1} A_k^T \text{ and } g_k = A_k H^{-1}(A_k^T y_k^c - g) - b_k$$

- apply conjugate-gradient method with safeguards to detect steps to infinity
- each matrix-vector product $H_k p$ requires solve with H and sparse matrix-vector products with A_k and A_k^T
- preconditioning possible but no obvious simple preconditioner

An example

POWELL20: $n = 10000, m = 10000$

- solve problem using interior-point package CQP from GALAHAD
- perturb constraints and resolve by dual gradient-projection DQP

	CQP	size of perturbation before DQP solve					
		0	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
time	4.60	0.03	0.13	0.41	1.92	9.21	7.94
its		0	1	1	15	32	35
changes		0	1	8	594	3506	4763

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`POWELL20`: $\mathbf{n = 10000, m = 10000}$

- solve problem using interior-point package `CQP` from GALAHAD
- perturb constraints and resolve by dual gradient-projection `DQP`

		size of perturbation before `DQP` solve					
	`CQP`	0	$\mathbf{10^{-6}}$	$\mathbf{10^{-5}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-2}}$
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Active-set changes per iteration with perturbation $\mathbf{10^{-2}}$:

584	285	245	345	331	340	332	297	291	255
249	223	223	213	207	197	205	192	166	146
129	123	133	134	124	115	114	114	107	87
63	44	16	1	0					

Summary

- dual gradient-projection method for large-scale, strictly-convex QP
- requires sparse factorization of Hessian but otherwise can be used "factorization-free"
- allows rapid change to the "active set"
- particularly suited to "warm starting"
- efficient projected search
- extensive use of Fredholm alternative
- many technical details
- easily generalised for regularization problems in ℓ_1 and ℓ_∞ norms using appropriate simple projections onto boxes and simplices
- implemented as a fortran 2003 module `DQP` in GALAHAD (G., Hogg, Scott)