INTERIOR POINT METHODS FOR LARGE-SCALE NONLINEAR PROGRAMMING

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Contents:

Nonlinear programming problem:

Consider the problem

$$\begin{array}{rcl} f(x) & \to & \min, \\ c_I(x) & \leq & 0, \\ c_E(x) & = & 0, \end{array}$$

$I = \{1, \ldots, m_I\}$, $E = \{m_I + 1, \ldots, m_I + m_E\}$, where functions $f(x)$, $c_I(x)$, $c_E(x)$ are twice continuously differentiable. Necessary (KKT) conditions have the following form (we assume the standard constraint qualifications):

$$\begin{array}{rcl} g(x,u) & = & 0, \\ c_I(x) & \leq & 0, \quad u_I \geq 0, \quad u_I^T c_I(x) = 0, \\ c_E(x) & = & 0, \end{array}$$

where

$$g(x,u) = \nabla f(x) + A_I(x) u_I + A_E(x) u_E,$$

and $A_I(x) = [\nabla c_i(x) : i \in I]$, $A_E(x) = [\nabla c_i(x) : i \in E]$. Here $u_I \in R^{m_I}$, $u_E \in R^{m_E}$ are vectors of Lagrange multipliers.

Interior point (IP) principle:

$$\begin{aligned} f(x) - \mu e^T \ln(S_I) e &\rightarrow \min, \\ c_I(x) + s_I &= 0, \\ c_E(x) &= 0, \end{aligned}$$

where $s_I > 0$ is a slack vector, e is the vector with unit elements and $S_I = \mathrm{diag}(s_i : i \in I)$ (we assume that $\mu \rightarrow 0$).

Necessary (KKT) conditions have the following form:

primal formulation	primal-dual formulation
$g(x, u) = 0,$	$g(x, u) = 0,$
$U_I e - \mu S_I^{-1} e = 0,$	$S_I U_I e - \mu e = 0,$
$c_I(x) + s_I = 0,$	$c_I(x) + s_I = 0,$
$c_E(x) = 0,$	$c_E(x) = 0,$

where

$$g(x, u) = \nabla f(x) + A_I(x) u_I + A_E(x) u_E,$$

and $S_I = \mathrm{diag}(s_i : i \in I)$, $U_I = \mathrm{diag}(u_i : i \in I)$. The inequalities $s_i > 0$ and $u_i > 0$ have to be satisfied in all iterations. Primal-dual formulation leads to more effective algorithms.

Direction determination (line-search approach):

Linearization - the Newton method

$$\begin{bmatrix} G & 0 & A_I & A_E \\ 0 & U_I & S_I & 0 \\ A_I^T & I & 0 & 0 \\ A_E^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta s_I \\ \Delta u_I \\ \Delta u_E \end{bmatrix} = - \begin{bmatrix} g \\ S_I U_I e - \mu e \\ c_I + s_I \\ c_E \end{bmatrix},$$

where $g = g(x, u)$ and

$$G = G(x, u) = \nabla^2 f(x) + \sum_{i \in I \cup E} u_i \nabla^2 c_i(x).$$

We assume that matrix of this system is nonsingular. Elimination of Δs_I:

$$\Delta s_I = -U_I^{-1} S_I (u_I + \Delta u_I) + \mu U_I^{-1} e$$

Active and inactive constraints ($\varepsilon_I > 0$).

$$\begin{aligned} \hat{s}_I \le \varepsilon_I \hat{u}_I \quad & - \quad \text{active constraints} \\ \check{s}_I > \varepsilon_I \check{u}_I \quad & - \quad \text{inactive constraints} \end{aligned}$$

Elimination of inactive constraints:

$$\Delta \check{u}_I = \check{S}_I^{-1} \check{U}_I (\check{c}_I + \check{A}_I^T \Delta x) + \mu \check{S}_I^{-1} e$$

The final equations

$$\begin{bmatrix} \hat{G} & \hat{A}_I & A_E \\ \hat{A}_I^T & -\hat{U}_I^{-1}\hat{S}_I & 0 \\ A_E^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \hat{u}_I \\ \Delta u_E \end{bmatrix} = - \begin{bmatrix} \hat{g} \\ \hat{c}_I + \mu \hat{U}_I^{-1} e \\ c_E \end{bmatrix},$$

where

$$\begin{aligned} \hat{G} &= G + \check{A}_I \check{S}_I^{-1} \check{U}_I \check{A}_I^T, \\ \hat{g} &= g + \check{A}_I \check{S}_I^{-1} \check{U}_I \check{c}_I + \mu \check{A}_I \check{S}_I^{-1} e. \end{aligned}$$

Both matrices $\hat{G}$ and $\hat{U}_I^{-1}\hat{S}_I$ are bounded (if G and A are bounded) and if the strict complementarity conditions hold, then $\lim_{\mu \to 0} \hat{U}_I^{-1}\hat{S}_I = 0$. After substitution we obtain

$$\begin{aligned} \Delta \hat{s}_I &= -\hat{U}_I^{-1}\hat{S}_I(\hat{u}_I + \Delta \hat{u}_I) + \mu \hat{U}_I^{-1} e, \\ \Delta \check{s}_I &= -(\check{c}_I + \check{A}_I^T \Delta x + \check{s}_I). \end{aligned}$$

Vector $\Delta \hat{u}_I$ is determined as an inexact solution of the above system, vector $\Delta \check{u}_I$ is obtained by direct elimination.

Indefinitely preconditioned conjugate gradient method:

$$K\bar{d} = \begin{bmatrix} \hat{G} & \hat{A} \\ \hat{A}^T & -\hat{M} \end{bmatrix} \begin{bmatrix} d \\ \hat{d} \end{bmatrix} = \begin{bmatrix} b \\ \hat{b} \end{bmatrix} = \bar{b},$$

where $\hat{A} = [\hat{A}_I, A_E]$ and $\hat{M} = \mathrm{diag}(\hat{M}_I, 0)$. Here $\hat{M}_I = \hat{U}_I^{-1}\hat{S}_I$ is a positive definite diagonal matrix. We assume that matrix K is nonsingular, which implies that A_E has a full column rank.

The first class of indefinite preconditioners:

$$C = \begin{bmatrix} \hat{D} & \hat{A} \\ \hat{A}^T & -\hat{M} \end{bmatrix},$$

where $\hat{D}$ is a positive definite diagonal matrix derived from the diagonal of $\hat{G}$. Expressions for matrices K and C imply that

$$C^{-1} = \begin{bmatrix} \hat{P} & \hat{Q} \\ \hat{Q}^T & -(\hat{A}^T\hat{D}^{-1}\hat{A} + \hat{M})^{-1} \end{bmatrix},$$

where $\hat{P} = \hat{D}^{-1} - \hat{D}^{-1}\hat{A}(\hat{A}^T\hat{D}^{-1}\hat{A} + \hat{M})^{-1}\hat{A}^T\hat{D}^{-1}$, $\hat{Q} = \hat{D}^{-1}\hat{A}(\hat{A}^T\hat{D}^{-1}\hat{A} + \hat{M})^{-1}$.

The preconditioned matrix

$$KC^{-1} = \left[\begin{array}{cc} I + (\hat{G} - \hat{D})\hat{P} & (\hat{G} - \hat{D})\hat{Q} \\ 0 & I \end{array} \right],$$

Basic theorems:

Theorem 1. Consider preconditioner C applied to system $K\bar{d} = \bar{b}$ and assume that $\hat{G} - \hat{D}$ is nonsingular. Then matrix KC^{-1} has at least $\hat{m}_I + 2m_E$ unit eigenvalues but at most $\hat{m}_I + m_E$ linearly independent eigenvectors corresponding to these eigenvalues exist. The other eigenvalues of matrix KC^{-1} are exactly eigenvalues of matrix $Z_E^T \tilde{G} Z_E (Z_E^T \tilde{D} Z_E)^{-1}$, where $[Z_E, A_E]$ is a nonsingular square matrix, $Z_E^T A_E = 0$, $Z_E^T Z_E = I$ and where

$$\begin{aligned} \tilde{G} &= \hat{G} + \hat{A}_I \hat{M}_I^{-1} \hat{A}_I^T, \\ \tilde{D} &= \hat{D} + \hat{A}_I \hat{M}_I^{-1} \hat{A}_I^T. \end{aligned}$$

If $Z_E^T \tilde{G} Z_E$ is positive definite then all eigenvalues are positive.

Theorem 2. Consider preconditioner C applied to system $K\bar{d} = \bar{b}$ and assume that $\hat{G} - \hat{D}$ is nonsingular. Then the Krylov subspace $\mathcal{K}$ defined by matrix KC^{-1} and vector $\bar{r} \in R^{n+\hat{m}_I+m_E}$, has a dimension of at most $\min(n+1, n-m_E+2)$.

The preconditioned CG method:

$$K\bar{d} = \begin{bmatrix} \hat{G} & \hat{A} \\ \hat{A}^T & -\hat{M} \end{bmatrix} \begin{bmatrix} d \\ \hat{d} \end{bmatrix} = \begin{bmatrix} b \\ \hat{b} \end{bmatrix} = \bar{b},$$

Algorithm PCG

$$\begin{array}{ll} d - \text{given}, & \hat{d} := 0, \\ r := b - \hat{G}d - \hat{A}\hat{d}, & \hat{r} := \hat{b} - \hat{A}^T d + \hat{M}\hat{d}, \\ \beta := 0, & \end{array}$$

while $\|r\| > \omega\|b\|$ or $\|\hat{r}\| > \omega\|\hat{b}\|$ **do**

$$\begin{array}{ll} \hat{t} := (\hat{A}^T\hat{D}^{-1}\hat{A} + \hat{M})^{-1}(\hat{A}^T\hat{D}^{-1}r - \hat{r}), & \\ t := \hat{D}^{-1}(r - \hat{A}\hat{t}), & \\ \gamma := r^T t + \hat{r}^T\hat{t}, & \beta := \beta\gamma, \\ p := t + \beta p, & \hat{p} := \hat{t} + \beta\hat{p}, \\ q := \hat{G}p + \hat{A}\hat{p}, & \hat{q} := \hat{A}^T p - \hat{M}\hat{p}, \\ \alpha := p^T q + \hat{p}^T\hat{q}, & \alpha := \gamma/\alpha, \\ d := d + \alpha p, & \hat{d} := \hat{d} + \alpha\hat{p}, \\ r := r - \alpha q, & \hat{r} := \hat{r} - \alpha\hat{q}, \\ \beta := 1/\gamma & \end{array}$$

end while.

Theorem 3. Consider Algorithm PCG with preconditioner C applied to system $K\bar{d} = \bar{b}$. Assume that initial $\bar{d}$ is chosen in such a way that $\hat{r} = 0$ at the start of the algorithm. Let matrix $Z_E^T \tilde{G} Z_E$ be positive definite. Then:

(a) Vector d^* (the first part of vector $\bar{d}^*$ which solves equation $K\bar{d} = \bar{b}$) is found after $n - m_E$ iterations at most.

(b) The algorithm cannot break down before d^* is found.

(c) Error $\|d - d^*\|$ converges to zero at least R - linearly with quotient

$$\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1},$$

where κ is the spectral condition number of matrix $Z_E^T \tilde{G} Z_E (Z_E^T \tilde{D} Z_E)^{-1}$.

(d) If $d = d^*$, then also $\hat{d}_I = \hat{d}_I^*$ and d_E^* can be determined by the formula

$$d_E^* = d_E + (A_E^T \tilde{D}^{-1} A_E)^{-1} A_E^T \tilde{D}^{-1} r.$$

Theorem 3 assumes that $\hat{r} = 0$ at the start of Algorithm PCG. This condition is satisfied if we set $\hat{d} = 0$ and

$$d = (\hat{A}^T \hat{D}^{-1} \hat{A})^{-1} \hat{A}^T \hat{D}^{-1} \hat{b}.$$

In Algorithm PCG, the sparse Choleski decomposition (complete or incomplete) of matrix $\hat{A}^T \hat{D}^{-1} \hat{A} + \hat{M}$ is used instead of its inversion. Unfortunately, this matrix can be dense if $\hat{A}$ has dense rows. Assume that $\hat{A}^T = [\hat{A}_s^T, \hat{A}_d^T]$ and $\hat{D} = \mathrm{diag}(\hat{D}_s, \hat{D}_d)$, where

$$\hat{M}_s = \hat{A}_s^T \hat{D}_s^{-1} \hat{A}_s + \hat{M}$$

is sparse and $\hat{A}_d$ consists of dense rows. Then

$$\begin{aligned}(\hat{A}^T \hat{D}^{-1} \hat{A} + \hat{M})^{-1} &= (\hat{M}_s + \hat{A}_d^T \hat{D}_d^{-1} \hat{A}_d)^{-1} \\ &= \hat{M}_s^{-1} - \hat{M}_s^{-1} \hat{A}_d^T \hat{M}_d^{-1} \hat{A}_d \hat{M}_s^{-1},\end{aligned}$$

where

$$\hat{M}_d = \hat{D}_d + \hat{A}_d \hat{M}_s^{-1} \hat{A}_d^T$$

is a (low-dimensional) dense matrix. Again the sparse Choleski decomposition of matrix $\hat{M}_s$ is used instead of its inversion.

Linear dependence of gradients of active constraints:

We use a perturbation of $\hat{M}$ to eliminate singularity (or near singularity) of matrix $\hat{A}^T\hat{D}^{-1}\hat{A}+\hat{M}$. Thus we solve equation

$$K\bar{d} = \begin{bmatrix} \hat{G} & \hat{A} \\ \hat{A}^T & -(\hat{M}+\hat{E}) \end{bmatrix} \begin{bmatrix} d \\ \hat{d} \end{bmatrix} = \begin{bmatrix} b \\ \hat{b} \end{bmatrix} = \bar{b}$$

and use preconditioner

$$C = \begin{bmatrix} \hat{D} & \hat{A} \\ \hat{A}^T & -(\hat{M}+\hat{E}) \end{bmatrix},$$

where $\hat{E}$ is a (small) positive semidefinite diagonal matrix.

Theorem 4. Let $\hat{d}(\varepsilon)$ be the solution of the perturbed system with $\hat{G}$ nonsingular and $\hat{E} = \varepsilon\hat{E}_0$. Then

$$\frac{1}{2}\frac{\mathrm{d}(\hat{d}^T(\varepsilon)\hat{E}_0\hat{d}(\varepsilon))}{\mathrm{d}\varepsilon} = \\ -\hat{d}^T(\varepsilon)\hat{E}_0(\hat{A}^T\hat{G}^{-1}\hat{A}+\hat{M}+\varepsilon\hat{E}_0)^{-1}\hat{E}_0\hat{d}(\varepsilon).$$

If there is a number $\overline{\varepsilon} \geq 0$ such that $\hat{A}^T\hat{G}^{-1}\hat{A} + \hat{M} + \varepsilon\hat{E}_0$ is positive definite $\forall\varepsilon \geq \overline{\varepsilon}$, the above expression is negative $\forall\varepsilon \geq \overline{\varepsilon}$ and $\hat{d}^T(\varepsilon)\hat{E}_0\hat{d}(\varepsilon) \to 0$ if $\varepsilon \to \infty$.

Regularization:

Matrix $\hat{C} = \hat{A}^T \hat{D}^{-1} \hat{A} + \hat{M}$ is at least positive semidefinite. We can use the Gill-Murray decomposition $\hat{R}^T \hat{R} = \hat{C} + \hat{E}$, where $\hat{R}$ is an upper triangular matrix and $\hat{E}$ is a small positive definite diagonal matrix. In the i-th elimination step, the pivot is changed so that

$$\hat{R}_{ii} = \max\left(|\hat{r}_{ii}|, \frac{\gamma_i}{\beta}, \delta \right),$$

where $\hat{r}_{ii}$ is the pivot before correction, $\beta^2 > \|\hat{C}\|$, $\delta = \sqrt{\varepsilon_M}\|\hat{C}\|$ (ε_M – machine precision) and γ_i is the maximum absolute value of the off diagonal element in the i-th row. Then $\hat{E}_{ii} = \hat{R}_{ii} - \hat{r}_{ii} \geq 0$. Then we obtain the reasonable preconditioner

$$C = \begin{bmatrix} \hat{D} & \hat{A} \\ \hat{A}^T & -(\hat{M} + \hat{E}) \end{bmatrix}$$

and the regularized system

$$\begin{bmatrix} \hat{G} & \hat{A} \\ \hat{A}^T & -(\hat{M} + \hat{E}) \end{bmatrix} \begin{bmatrix} d \\ \hat{d} \end{bmatrix} = \begin{bmatrix} b \\ \hat{b} \end{bmatrix}.$$

Another possibility is to compute an approximation $\underline{\lambda}$ of the least eigenvalue of $\hat{C}$ (from the Choleski decomposition) and replace M by $M + \delta I$ if $\underline{\lambda} \leq \delta$.

Additional indefinite preconditioners:

Let

$$C = \left[\begin{array}{cc} \hat{B} & \hat{A} \\ \hat{A}^T & -\hat{N} \end{array} \right],$$

where $\hat{N} = \hat{M} + \hat{D} - \nu \hat{A}^T \hat{B}^{-1} \hat{A}$, $\hat{B}$ is a nonsingular approximation of $\hat{G}$ (usually $\hat{B} = \hat{G}$), $\hat{D}$ is a diagonal matrix such that $\hat{M} + \hat{D}$ is positive definite and ν is a parameter. Using $\hat{B}$ or $\hat{N}$ for block elimination, we obtain

$$C^{-1} = \begin{array}{cc} \hat{B}^{-1} - \hat{B}^{-1} \hat{A} \hat{C}^{-1} \hat{A}^T \hat{B}^{-1} & \hat{B}^{-1} \hat{A} \hat{C}^{-1} \\ \hat{C}^{-1} \hat{A}^T \hat{B}^{-1} & -\hat{C}^{-1} \end{array} ,$$

where $\hat{C} = \hat{A}^T \hat{B}^{-1} \hat{A} + \hat{N}$ ($\hat{C} = \hat{M} + \hat{D}$ if $\nu = 1$), or

$$C^{-1} = \begin{array}{cc} \tilde{B}^{-1} & \tilde{B}^{-1} \hat{A} \hat{N}^{-1} \\ \hat{N}^{-1} \hat{A}^T \tilde{B}^{-1} & \hat{N}^{-1} \hat{A}^T \tilde{B}^{-1} \hat{A} \hat{N}^{-1} - \hat{N}^{-1} \end{array} ,$$

where $\tilde{B} = \hat{B} + \hat{A} \hat{N}^{-1} \hat{A}^T$ ($\hat{N} = \hat{M} + \hat{D}$ if $\nu = 0$). Matrix $\tilde{B}$ is usually sparse (it is dense when $\hat{A}$ has dense columns). If $\hat{B} = \hat{G}$, then

$$K C^{-1} = \left[\begin{array}{cc} I & 0 \\ (I - \hat{H}) \hat{A}^T \hat{G}^{-1} & \hat{H} \end{array} \right],$$

where $\hat{H} = (\hat{A}^T \hat{G}^{-1} \hat{A} + \hat{M}) \hat{C}^{-1}$. Notice that $\hat{H} = \hat{A}^T \tilde{B}^{-1} \hat{A} \hat{N}^{-1}$ if $\hat{M} = 0$.

Theorem 5. Consider preconditioner C with $\hat{B} = \hat{G}$ and $\hat{M} + \hat{D}$ positive definite applied to system $K\bar{d} = \bar{b}$. Then matrix KC^{-1} has at least n unit eigenvalues with a full system of n linearly independent eigenvectors. The other eigenvalues of KC^{-1} are exactly eigenvalues of matrix $\hat{H} = (\hat{A}^T\hat{G}^{-1}\hat{A} + \hat{M})\hat{C}^{-1}$. If $\hat{A}^T\hat{G}^{-1}\hat{A} + \hat{M}$ is positive definite then all eigenvalues are positive.

Theorem 6. Consider preconditioner C with $\hat{B} = \hat{G}$ applied to system $K\bar{d} = \bar{b}$. Then the Krylov subspace $\mathcal{K}$ defined by matrix KC^{-1} and vector $\bar{r} \in R^{n+\hat{m}}$, has a dimension of at most $\hat{m} + 1$.

Theorem 7. Consider the conjugate gradient method preconditioned by C with $\hat{B} = \hat{G}$ and applied to system $K\bar{d} = \bar{b}$. Assume that initial $\bar{d}$ is chosen in such a way that $r = 0$ at the start of the algorithm. Let matrix $\hat{A}^T\hat{G}^{-1}\hat{A} + \hat{M}$ be positive definite. Then:

(a) Vector $\bar{d}^*$ which solves equation $K\bar{d} = \bar{b}$ is found after $\hat{m}$ iterations at most.

(b) The algorithm cannot break down before $\bar{d}^*$ is found.

(c) Error $\|\hat{d} - \hat{d}^*\|$ converges to zero at least R - linearly with quotient $(\sqrt{\kappa} - 1)/(\sqrt{\kappa} + 1)$, where κ is the spectral condition number of matrix $\hat{H} = (\hat{A}^T\hat{G}^{-1}\hat{A} + \hat{M})\hat{C}^{-1}$.

Strategies for step-length restriction:

Let $x_+ = x + \alpha\Delta x$, where $0 < \alpha < \overline{\alpha}$ with $\overline{\alpha} = \min(1, \overline{\Delta}/\|\Delta x\|)$. Since $s_I^+ > 0$ and $u_I^+ > 0$ have to hold, step-lengths for s_I and u_I have to be restricted. Strategy 1 uses individual step-lengths $s_i^+ = s_i + \alpha_{s_i}\Delta s_i$ and $u_i^+ = u_i + \alpha_{u_i}\Delta u_i$, where

$$\alpha_{s_i} = \alpha, \qquad \Delta s_i \geq 0,$$

$$\alpha_{s_i} = \min\left(\alpha, -\gamma\frac{s_i}{\Delta s_i}\right), \qquad \Delta s_i < 0,$$

$$\alpha_{u_i} = \alpha, \qquad \Delta u_i \geq 0,$$

$$\alpha_{u_i} = \min\left(\alpha, -\gamma\frac{u_i}{\Delta u_i}\right), \qquad \Delta u_i < 0,$$

($0 < \gamma < 1$ is a coefficient close to unit). Other strategies require bounds

$$\begin{aligned}
\overline{\alpha}_s &= \gamma \min_{i \in I, \Delta s_i < 0}\left(-\frac{s_i}{\Delta s_i}\right), \\
\overline{\alpha}_u &= \gamma \min_{i \in I, \Delta u_i < 0}\left(-\frac{u_i}{\Delta u_i}\right),
\end{aligned}$$

where $0 < \gamma < 1$ and define

$$\begin{aligned}
s_I^+ = s_I(\alpha) &= s_I + \min(\alpha, \overline{\alpha}_s)\Delta s_I, \\
u_I^+ = u_I(\alpha) &= u_I + \min(\alpha, \overline{\alpha}_u)\Delta u_I.
\end{aligned}$$

Merit function for step-length selection:

$$\begin{aligned}
P(\alpha) &= f(x+\alpha\Delta x) - \mu e^T \ln(S_I(\alpha))e \\
&+ (u_I + \Delta u_I)^T (c_I(x+\alpha\Delta x) + s_I(\alpha)) \\
&+ (u_E + \Delta u_E)^T c_E(x+\alpha\Delta x) \\
&+ \frac{\sigma}{2}\|c_I(x+\alpha\Delta x) + s_I(\alpha) - E_I(u_I(\alpha) - u_I)\|^2 \\
&+ \frac{\sigma}{2}\|c_E(x+\alpha\Delta x) - E_E\alpha\Delta u_E\|^2,
\end{aligned}$$

where $\sigma \geq 0$.

Theorem 8. Let $s_I > 0$, $u_I > 0$ and let the triple Δx, $\Delta\hat{u}_I$, Δu_E be an inexact solution of a regularized system. Then

$$\begin{aligned}
P'(0) &= -(\Delta x)^T G\Delta x - (\Delta s_I)^T S_I^{-1} U_I \Delta s_I \\
&- \sigma(\|c_I + s_I\|^2 + \|c_E\|^2) \\
&+ (\Delta x)^T r + \sigma((\hat{c}_I + \hat{s}_I)^T \hat{r}_I + c_E^T r_E).
\end{aligned}$$

where r, $\hat{r}_I$, r_E are parts of the residual vector. If

$$\sigma > -\frac{(\Delta x^T)G\Delta x + (\Delta s_I)^T S_I^{-1} U_I \Delta s_I}{\|c_I + s_I\|^2 + \|c_E\|^2}$$

and if $(\Delta x)^T r + \sigma((\hat{c}_I + \hat{s}_I)^T \hat{r}_I + c_E^T r_E)$ is sufficiently small, then

$$P'(0) < 0$$

.

Restart:

If $P'(0) \geq 0$, then line-search usually fails. There are two basic possibilities.

- We recompute $\sigma \geq 0$ so that

$$\sigma > -\frac{(\Delta x^T)G\Delta x + (\Delta s_I)^T S_I^{-1} U_I \Delta s_I}{\|c_I + s_I\|^2 + \|c_E\|^2}.$$

  Then $P'(0) < 0$.

- We keep $\sigma \geq 0$ unchanged, replace matrix $\hat{G}$ by a positive definite diagonal matrix $\hat{D}$ and resolve the resulting linear system. Moreover, we use the same diagonal matrix for the construction of the first-type preconditioner.

Theorem 9. Consider Algorithm PCG with preconditioner C applied to system $K\bar{d} = \bar{b}$ (with $\hat{G}$ replaced by $\hat{D}$). Then this algorithm finds the exact solution in its first iteration and $P'(0) < 0$ for any value $\sigma \geq 0$.

The use of restarts is computationally more efficient than the recomputation of $\sigma \geq 0$.

Computation of the barrier parameter

Most implementations of interior-point methods choose the value μ in such a way that

$$0 < \mu < s_I^T u_I / m_I$$

(or $\mu = \lambda s_I^T u_I / m_I$, where $0 < \lambda < 1$). Computational experience indicates that the algorithm performs best when components $s_i u_i$ approach zero at a uniform rate. The distance from uniformity can be measured by the ratio

$$\varrho = \frac{\min_{i \in I}(s_i u_i)}{s_I^T u_I / m_I}$$

(the centrality measure). Clearly, $0 < \varrho \leq 1$ and $\varrho = 1$ if and only if $S_I U_I e = \mu e$. The value λ is then computed by using ϱ. Usually heuristic formulas are used for this purpose. In our implementation, we have used the formula

$$\lambda = 0.1 \min \left(0.05 \frac{1 - \varrho}{\varrho}, 2 \right)^3$$

proposed by Vanderbei and Shanno. We have also tested other possibilities, e.g., formulas given by Argaez, Tapia and Velasquez, but the above formula has shown to be best.

Numerical experiments:

Interior-point method was tested by using three sets each containing 17 test problems with 1000 variables. The results are listed in three tables, where:

- M - method for step-length selection (F - the first step accepted, L - line search).
- S - strategy for step-length restriction.
- P - the preconditioner used (the first and the second classes with complete (+) or incomplete (-) Gill-Murray decomposition).
- NIT - the total number of iterations.
- NFV - the total number of function evaluations.
- NFG - the total number of gradient evaluations (NFG is much greater than NIT, since the second order derivatives are computed by using gradient differences)
- NCG - the total number of CG iterations.
- NRS - the total number of restarts.
- NFAIL - the number of failures for a given set (the number of problems which have not been solved).

M	S	P	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
F	1	1	567	567	4137	24969	20	4.88	-
F	2	1	529	529	3855	23473	14	4.75	-
F	3	1	611	611	4680	25431	22	5.92	-
L	1	1	508	711	3832	24933	20	5.28	-
L	2	1	550	593	3936	21806	14	4.67	-
L	3	1	622	695	4785	22801	27	5.92	-
F	1	1	567	567	4137	24969	20	4.88	-
F	1	-1	549	549	3954	25021	17	4.94	-
F	1	2	1037	1038	6986	3166	23	4.48	1
F	1	-2	1726	1727	12120	9315	170	18.11	1
L	2	1	550	593	3936	21806	14	4.64	-
L	2	-1	575	761	4127	24101	18	5.17	1
L	2	2	781	1770	5776	2150	15	4.28	1
L	2	-2	845	2041	6922	18061	25	13.86	2

Table 1: Set 1 of 17 problems with 1000 variables

M	S	P	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
F	1	1	393	393	2823	10728	19	2.88	-
F	2	1	413	413	2994	5435	19	2.67	-
F	3	1	672	672	4896	9964	12	4.03	-
L	1	1	395	846	2812	16396	72	4.09	1
L	2	1	476	925	3403	5654	73	3.28	1
L	3	1	876	1343	6223	17823	69	6.14	1
F	1	1	393	393	2823	10728	19	2.88	-
F	1	-1	388	388	2790	11513	10	3.06	-
F	1	2	908	908	5952	1091	14	4.64	-
F	1	-2	860	860	5661	6231	7	9.80	-
L	2	1	476	925	3403	5654	73	3.28	1
L	2	-1	482	939	3449	6521	72	3.57	1
L	2	2	911	1597	6067	2275	52	5.14	2
L	2	-2	902	1691	6079	2937	65	10.07	2

Table 2: Set 2 of 17 problems with 1000 variables (problems LUKVLI1–LUKVLI18 from CUTE)

M	S	P	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
F	1	1	550	551	3895	2737	11	5.75	1
F	2	1	567	567	4114	2993	6	5.69	-
F	3	1	737	751	5347	5342	28	8.84	2
L	1	1	471	694	3502	4492	26	6.25	1
L	2	1	540	637	4070	3475	21	6.67	-
L	3	1	941	1311	7448	15261	45	12.92	2
F	1	1	550	551	3895	2738	11	5.75	1
F	1	-1	542	548	3850	3204	12	8.78	1
F	1	2	541	541	3861	3790	29	5.34	1
F	1	-2	502	502	3529	942	14	5.64	1
L	2	1	540	637	4070	3475	21	6.67	-
L	2	-1	546	688	4125	3532	21	7.86	-
L	2	2	495	705	3699	745	22	4.31	-
L	2	-2	467	709	3321	983	29	6.33	1

Table 3: Set 3 of 17 problems with 1000 variables

The CUTE[1] collection:

Problem	n	m	S	P	NIT	NFV	NFG	NCG
BRITGAS	450	360	1	1	15	15	285	132
CLNLBEAM	1503	1000	1	1	19	19	133	81
DALLASL	906	667	1	1	47	47	893	47
EG3	1001	2000	3	-1	41	41	287	251
EIGENB2	420	210	1	1	8	8	3261	207
EIGENC2	462	231	1	1	17	17	7531	180
GAUSSELM	819	1296	3	1	20	20	660	1640
HANGING	1800	1150	1	1	29	29	609	792
MANNE	600	400	3	-1	50	50	300	476
NGONE	100	1273	3	-1	35	35	3535	539
OPTCDEG2	1202	800	1	1	11	11	88	236
OPTCDEG3	1202	800	1	1	7	7	56	11
OPTMASS	1210	1005	1	1	6	6	48	26
READING1	2002	1000	3	-1	35	35	245	352
READING3	2002	1001	3	-1	19	19	133	532
READING4	1001	1000	3	-2	51	51	204	73
READING5	5001	5000	1	-1	2	3	12	4
READING9	2002	1000	1	1	11	11	55	53
SINROSNB	1000	999	1	1	13	13	52	50
SREADIN3	1002	501	1	-1	38	38	266	193
SSNLBEAM	3003	2000	1	1	19	19	133	125
SVANBERG	1000	1000	1	1	20	20	380	81
TRAINF	2008	1002	1	1	37	37	370	94
TRAINH	2008	1002	1	1	30	30	390	424
ZAMB2	1326	480	1	-1	29	29	348	1927

Table 4 : The first step accepted (M = F)

[1] N.I.M. Gould, D. Orban, P.L.Toint: CUTEr (and SifDec), a Constrained and Unconstrained Testing Environment, revisited.

The comparison with NITRO[2]:

	Algorithm 1			NITRO		
Problem	n	m	**NFV**	n	m	**NFV**
CLNLBEAM	1503	1000	19	303	200	21
DALLASL	906	667	47	906	667	100
EG3	1001	2000	41	101	200	31
GAUSSELM	819	1926	22	819	1926	115
GRIDNETA	924	484	12	924	484	21
GRIDNETD	924	484	12	924	484	19
GRIDNETF	924	484	17	924	484	20
GRIDNETG	924	484	13	924	484	21
GRIDNETI	924	484	15	924	484	28
MANNE	600	400	50	300	200	9
NGONE	100	1273	35	100	1273	217
OPTCDEG2	1202	800	11	302	200	30
OPTCDEG3	1202	800	7	302	200	22
OPTMASS	1210	1005	6	610	505	15
READING1	2002	1000	35	202	100	52
READING3	2002	1001	19	303	200	12
READING4	1001	1000	51	202	101	77
READING5	5001	5000	3	501	500	6
READING9	2002	1000	11	501	500	15
SINROSNB	1000	999	13	1000	999	90
SREADIN3	1002	501	38	202	101	30
SSNLBEAM	3003	2000	19	303	200	23
SVANBERG	1000	1000	20	1000	1000	18
TRAINF	2008	1002	34	808	402	345
TRAINH	2008	1002	30	808	402	441
ZAMB2	1326	480	29	1326	480	37

Table 5 : Comparison of results

[2] **R.H Byrd, J. Nocedal, R.A.Waltz: Feasible Interior Methods Using Slacks for Nonlinear Optimization.**

Direction determination (trust-region approach):

Linearization - the Newton method (after elimination of inactive constraints). Only active slacks are considered in the trust-region subproblem. Primal-dual formulation is used.

$$\begin{bmatrix} \hat{G} & 0 & \hat{A}_I & A_E \\ 0 & \hat{S}_I^{-1}\hat{U}_I & I & 0 \\ \hat{A}_I^T & I & 0 & 0 \\ A_E^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \hat{s}_I \\ \Delta \hat{u}_I \\ \Delta u_E \end{bmatrix} = - \begin{bmatrix} \hat{g} \\ \hat{g}_s \\ \hat{c}_I + \hat{s}_I \\ c_E \end{bmatrix},$$

where $\hat{g}_s = \hat{u}_I - \mu \hat{S}_I^{-1} e$ and

$$\begin{aligned} \hat{G} &= G + \check{A}_I \check{S}_I^{-1} \check{U}_I \check{A}_I^T, \\ \hat{g} &= g + \check{A}_I \check{S}_I^{-1} \check{U}_I \check{c}_I + \mu \check{A}_I \check{S}_I^{-1} e, \end{aligned}$$

Scaling

$$\begin{bmatrix} \hat{G} & 0 & \hat{A}_I & A_E \\ 0 & I & \hat{D}_I & 0 \\ \hat{A}_I^T & \hat{D}_I & 0 & 0 \\ A_E^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \hat{D}_I^{-1} \Delta \hat{s}_I \\ \Delta \hat{u}_I \\ \Delta u_E \end{bmatrix} = - \begin{bmatrix} \hat{g} \\ \hat{D}_I \hat{g}_s \\ \hat{c}_I + \hat{s}_I \\ c_E \end{bmatrix},$$

where $\hat{D}_I = \sqrt{\hat{S}_I^{-1}\hat{U}_I}$. Notation

$$\bar{G} = \begin{bmatrix} \hat{G} & 0 \\ 0 & I \end{bmatrix}, \; \bar{g} = \begin{bmatrix} \hat{g} \\ \hat{D}_I \hat{g}_s \end{bmatrix}, \; \Delta z = \begin{bmatrix} \Delta x \\ \hat{D}_I^{-1} \Delta \hat{s}_I \end{bmatrix}.$$

Trust region subproblem:

$$\begin{aligned} \frac{1}{2}(\Delta z)^T \bar{G} \Delta z + \bar{g} \Delta z &\rightarrow \min, \\ \hat{A}^T \Delta z + \hat{c} &= 0, \\ \|\Delta z\| &\leq \Delta, \end{aligned}$$

(with the additional constraint $\hat{s}_I + \Delta \hat{s}_I > 0$), where

$$\hat{A} = \begin{bmatrix} \hat{A}_I & A_E \\ \hat{D}_I & 0 \end{bmatrix}, \; \hat{c} = \begin{bmatrix} \hat{c}_I + \hat{s}_I \\ c_E \end{bmatrix}, \; \Delta \hat{u} = \begin{bmatrix} \Delta \hat{u}_I \\ \Delta u_E \end{bmatrix}.$$

The Byrd-Omojokun approach: $\Delta z = \Delta z_V + \Delta z_H$.

Vertical subproblem:

$$\begin{aligned} \|\hat{A}^T \Delta z_V + \hat{c}\| &\rightarrow \min, \\ \|\Delta z_V\| &\leq \delta \Delta, \end{aligned}$$

where $0 < \delta < 1$. Horizontal subproblem:

$$\begin{aligned} \frac{1}{2}(\Delta z_H)^T \bar{G} \Delta z_H + (\bar{g} + \bar{G} \Delta z_V)^T \Delta z_H &\rightarrow \min, \\ \hat{A}^T \Delta z_H &= 0, \\ \|\Delta z_H\|^2 + \|\Delta z_V\|^2 &\leq \Delta^2. \end{aligned}$$

The additional constraint $\hat{s}_I + \Delta \hat{s}_I > 0$ has to be taken into account.

Vertical step:

$$\begin{aligned}\Delta z_V^C &= -\frac{\|\hat{A}\hat{c}\|}{\|\hat{A}^T\hat{A}\hat{c}\|}\hat{A}\hat{c},\\ \Delta z_V^N &= -\hat{A}(\hat{A}^T\hat{A})^{-1}\hat{c}\end{aligned}$$

(Δz_V^C - The Cauchy step, Δz_V^N - The Newton step).

The dog-leg method:

- If $\|\Delta z_V^C\| \geq \delta\Delta$, then $\Delta z_V = \frac{\delta\Delta}{\|\Delta z_V^C\|}\Delta z_V^C$.

- If $\|\Delta z_V^N\| \leq \delta\Delta$, then $\Delta z_V = \Delta z_V^N$.

- If $\|\Delta z_V^C\| < \delta\Delta < \|\Delta z_V^N\|$, then

$$\Delta z_V = \Delta z_V^C + \alpha(\Delta z_V^N - \Delta z_V^C)$$

where α is chosen so that $\|\Delta z_V\| = \delta\Delta$.

The additional constraint $\Delta\hat{s}_I \geq 0$ can imply an additional decrease of the step-length.

Horizontal step:

$$\hat{A}^T \Delta z_H = 0 \;\Rightarrow\; \Delta z_H = \hat{Z} \Delta z_Z,$$

where columns of $\hat{Z}$ form a basis in the null-space of $\hat{A}^T$. Then

$$\begin{aligned} \frac{1}{2}(\Delta z_Z)^T \hat{Z}^T \bar{G} \hat{Z} \Delta z_Z + \bar{g}_H^T \hat{Z} \Delta z_H \quad &\rightarrow \quad \min, \\ \|\hat{Z} \Delta z_Z\|^2 + \|\Delta z_V\|^2 \quad &\leq \quad \Delta^2, \end{aligned}$$

where $\bar{g}_H = \bar{g} + \bar{G} \Delta z_V$. This is an unconstrained trust region subproblem, which can be solved by the Steihaug-Toint CG method (preconditioned by $\hat{Z}^T \hat{Z}$). The use of $\Delta z_H = \hat{Z} \Delta z_Z$ (instead of Δz_Z) leads to the multiplication by the matrix

$$\hat{Z}(\hat{Z}^T \hat{Z})^{-1} \hat{Z}^T = I - \hat{A}(\hat{A}^T \hat{A})^{-1} \hat{A}^T.$$

Thus matrix $\hat{Z}$ need not be computed. Notice that the preconditioner

$$\hat{A}^T \hat{A} = \begin{bmatrix} \hat{A}_I^T \hat{A}_I + \hat{D}_I^2 & \hat{A}_I^T A_E \\ A_E^T \hat{A}_I & A_E^T A_E \end{bmatrix}$$

(where $\hat{D}_I^2 = \hat{S}_I^{-1} \hat{U}_I$) is the same as that used in line-search methods (this is the reason for our choice of $\hat{D}_I$). Solution of the horizontal subproblem gives $\Delta \hat{u}$ as a by-product.

Step-length restriction:

After determination $\Delta\hat{s}_I$ and $\Delta\hat{u}_I$ from the Byrd-Omojokun trust-region subproblem ve set

$$
\begin{aligned}
\Delta\check{s}_I &= -(\check{c}_I + \check{A}_I^T \Delta x + \check{s}_I), \\
\Delta\check{u}_I &= \check{S}_I^{-1}\check{U}_I(\check{c}_I + \check{A}_I^T \Delta x) + \mu \check{S}_I^{-1} e.
\end{aligned}
$$

Since $s_I^+ > 0$ and $u_I^+ > 0$ have to hold, step-lengths for s_I and u_I have to be restricted. we use the bounds

$$
\begin{aligned}
\overline{\alpha}_s &= \gamma \min_{i \in I, \Delta s_i < 0} \left(-\frac{s_i}{\Delta s_i} \right), \\
\overline{\alpha}_u &= \gamma \min_{i \in I, \Delta u_i < 0} \left(-\frac{u_i}{\Delta u_i} \right),
\end{aligned}
$$

where $0 < \gamma < 1$ and define $x^+ = x + \Delta x$, $s_I^+ = s_I(1)$, $u_I^+ = u_I(1)$, $u_E^+ = u_E + \Delta u_E$, where

$$
\begin{aligned}
s_I(\alpha) &= s_I + \min(\alpha, \overline{\alpha}_s) \Delta s_I, \\
u_I(\alpha) &= u_I + \min(\alpha, \overline{\alpha}_u) \Delta u_I.
\end{aligned}
$$

Notice that the step-length for $\hat{s}_I^+$ is usually restricted by using additional constraints in the Byrd-Omojokun trust-region subproblem.

Merit function for trust-region reduction:

$$
\begin{aligned}
P(\alpha) &= f(x+\alpha\Delta x) - \mu e^T \ln(S_I(\alpha))e \\
&+ (u_I + \Delta u_I)^T (c_I(x+\alpha\Delta x) + s_I(\alpha)) \\
&+ (u_E + \Delta u_E)^T c_E(x+\alpha\Delta x) \\
&+ \frac{\sigma}{2}\|c_I(x+\alpha\Delta x) + s_I(\alpha)\|^2 \\
&+ \frac{\sigma}{2}\|c_E(x+\alpha\Delta x)\|^2,
\end{aligned}
$$

where $\sigma \geq 0$. Obviously,

$$P'(0) = (\Delta z)^T(\bar{g} + \hat{A}\Delta\hat{u} + \sigma\hat{A}\hat{c}).$$

Theorem 10. Denote by

$$Q(\alpha) = P(0) + \alpha P'(0) + \frac{\alpha^2}{2}(\Delta z)^T \bar{G}\Delta z$$

the quadratic approximation of $P(\alpha)$. Let Δz be the solution of the Byrd-Omojokun trust-region subproblem (with residual vector $\hat{r} = \hat{A}^T\Delta z + \hat{c}$ such that $\|\hat{r}\| < \|\hat{c}\|$) and let

$$\sigma > \frac{(\Delta z)^T(\bar{g} + \hat{A}\Delta\hat{u}) + \frac{1}{2}(\Delta z)^T\bar{G}\Delta z}{\hat{c}^T(\hat{c} - \hat{r})},$$

then $Q(1) < Q(0)$.

Trust region strategy:

- We compute Δz by using the Byrd-Omojokun trust-region subproblem. Then either $\|\Delta z\| = \Delta$ or the horizontal subproblem is solved with a sufficient precision.

- We set $x^+ = x + \Delta x$, $s_I^+ = s_I(1)$, $u_I^+ = u_I(1)$, $u_E^+ = u_E + \Delta u_E$ if $P(1) < P(0)$ and $x^+ = x$, $s_I^+ = s_I$, $u_I^+ = u_I$, $u_E^+ = u_E$ otherwise.

- Denoting
$$\rho = \frac{P(1) - P(0)}{Q(1) - Q(0)},$$
we set
$$\begin{aligned} \Delta^+ = \beta\|\Delta z\| \quad &\text{if} \quad \rho < \underline{\rho}, \\ \Delta^+ = \Delta \quad &\text{if} \quad \underline{\rho} \le \rho \le \overline{\rho}, \\ \Delta^+ = \gamma\Delta \quad &\text{if} \quad \overline{\rho} < \rho. \end{aligned}$$

Here $0 < \beta < 1 < \gamma$ and $0 < \underline{\rho} < \overline{\rho} < 1$.

M	S	P	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
L	1	1	567	567	4137	24969	20	4.88	-
L	2	1	550	593	3936	21806	14	4.67	-
T	1	1	1344	1431	11995	18188	16	9.38	1
T	2	1	1106	1171	8522	26060	10	10.53	1

Table 6: Set 1 of 17 problems with 1000 variables

M	S	P	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
L	1	1	393	393	2823	10728	19	5.75	-
L	2	1	476	925	3403	5654	73	6.67	1
T	1	1	906	941	6048	10448	1	5.84	1
T	2	1	904	998	6185	10521	8	6.77	1

Table 7: Set 2 of 17 problems with 1000 variables (problems LUKVLI1–LUKVLI18 from CUTE)

M	S	P	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
L	1	1	550	551	3895	2737	11	5.75	1
L	2	1	540	637	4070	3475	21	6.67	-
T	1	1	697	768	5133	5925	0	8.72	1
T	2	1	544	625	3989	7545	8	8.36	1

Table 8: Set 3 of 17 problems with 1000 variables