An optimal algorithm with Barzilai-Borwein steplength and superrelaxation for QPQC problem

[Panm16]

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Osnova prezentace

- Motivace (kontaktní úloha s daným třením)
- QPQC
- stávající algoritmy (MPGP, SPG)
- modifikace (MPGP-BB)
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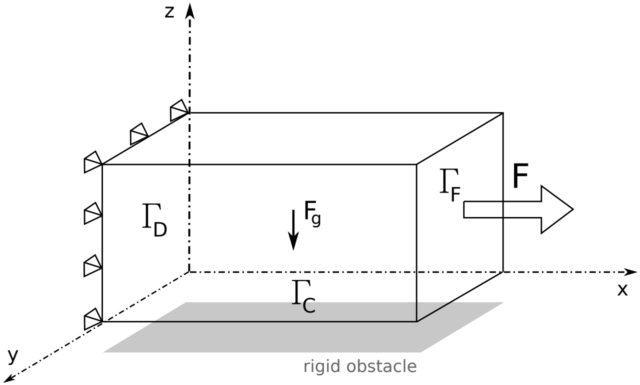
- několik poznámek ke konvergenci
- závěr

Kontaktní úloha s daným třením



Primární úloha

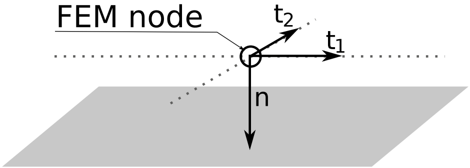
Nalezněte

$$\bar{\mathbf{u}} := \arg\min_{\mathbf{u}\in\Omega_C} f(\mathbf{u}) + j_h(\mathbf{u})$$

kde

- $\Omega_C := \{\mathbf{u} \in \Gamma_C : u_z \geq -d_C\}$,
- $f(\mathbf{u}) := 1/2\langle \mathbf{K}\mathbf{u}, \mathbf{u}\rangle - \langle \mathbf{f}, \mathbf{u}\rangle, f : \mathbb{R}^n \to \mathbb{R}$,
- $j_h(\mathbf{u}) := \sum_{i=1}^{m_c} \psi_i \|\mathbf{T}_i\mathbf{u}\|, j_h : \mathbb{R}^n \to \mathbb{R}$.

Tření a tečné vektory

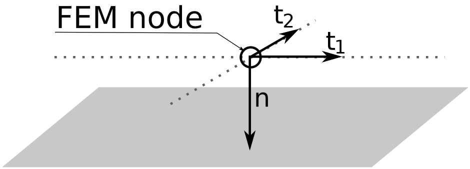


$$\mathbf{T}_i := \begin{bmatrix} 0 & 0 & 0 & \dots & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{T} := \left[\mathbf{T}_1^T, \dots, \mathbf{T}_{m_c}^T\right]^T$$

$$j_h(\mathbf{u}) := \sum_{i=1}^{m_c} \psi_i \|\mathbf{T}_i\mathbf{u}\| = \sum_{i=1}^{m_c} \max_{\|\tau_i\| \le \psi_i} \boldsymbol{\tau}_i^T \mathbf{T}_i \mathbf{u}$$

Podmínky nepronikání a normálové vektory



$$r_i^{\mathbf{B}} := \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & -1 & \dots & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{c}_i := d_C$$

$$\mathbf{Bu} \leq \mathbf{c}$$

Duální úloha

Z primární úlohy

$$\min_{\mathbf{u}\in\Omega_C}\left(f(\mathbf{u})+\sum_{i=1}^{m_c}\max_{\|\tau_i\|\le\psi_i}\boldsymbol{\tau}_i^T\mathbf{T}_i\mathbf{u}\right)$$

vytvořením nových Lagrangeových multiplikátorů

$$\min_{\mathbf{u}\in\mathbb{R}^n}\sup_{[\tau,\boldsymbol{\lambda}_C]\in\Lambda} f(\mathbf{u})+\boldsymbol{\tau}^T\mathbf{T}\mathbf{u}+\boldsymbol{\lambda}_C^T(\mathbf{B}\mathbf{u}-\mathbf{c}),$$

kde

$$\Lambda:=\{[\boldsymbol{\tau},\boldsymbol{\lambda}_C]\in\mathbb{R}^{3m_c}:\sqrt{\tau_{2i-1}^2+\tau_{2i}^2}\le\psi_i, i=1,\dots,m_c,\boldsymbol{\lambda}_C\ge\mathbf{o}\}.$$

Dále pak

$$\min_{\mathbf{u}\in\mathbb{R}^n}\sup_{\boldsymbol{\lambda}\in\Lambda} f(\mathbf{u})+\boldsymbol{\lambda}^T(\tilde{\mathbf{B}}\mathbf{u}-\tilde{\mathbf{c}})=:\min_{\mathbf{u}\in\mathbb{R}^n}\sup_{\boldsymbol{\lambda}\in\Lambda} L(\mathbf{u},\boldsymbol{\lambda}),$$

kde

$$\boldsymbol{\lambda}:=\begin{bmatrix}\boldsymbol{\tau}\\ \boldsymbol{\lambda}_C\end{bmatrix},\quad \tilde{\mathbf{B}}:=\begin{bmatrix}\mathbf{T}\\ \mathbf{B}\end{bmatrix},\quad \tilde{\mathbf{c}}:=\begin{bmatrix}\mathbf{o}\\ \mathbf{c}\end{bmatrix}.$$

Duální úloha

$$\min_{\mathbf{u}\in\mathbb{R}^n} \sup_{\boldsymbol{\lambda}\in\Lambda} L(\mathbf{u},\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda}\in\Lambda} \min_{\mathbf{u}\in\mathbb{R}^n} L(\mathbf{u},\boldsymbol{\lambda}).$$

Z první KKT podmínky

$$\begin{aligned} \mathbf{K}\mathbf{u} - \mathbf{f} + \tilde{\mathbf{B}}^T\boldsymbol{\lambda} &= \mathbf{o} \\ \mathbf{u} &= \mathbf{K}^{-1}\left(\mathbf{f} - \tilde{\mathbf{B}}^T\boldsymbol{\lambda}\right). \end{aligned}$$

Dosazením

$$L(\mathbf{u},\boldsymbol{\lambda}) = -\frac{1}{2}\boldsymbol{\lambda}^T\tilde{\mathbf{B}}\mathbf{K}^{-1}\tilde{\mathbf{B}}^T\boldsymbol{\lambda} + \boldsymbol{\lambda}^T(\tilde{\mathbf{B}}\mathbf{K}^{-1}\mathbf{f} - \tilde{\mathbf{c}}) - \frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f}.$$

Duální úloha má tvar

$$\bar{\boldsymbol{\lambda}} = \arg\min_{\lambda\in\Lambda} \Theta(\boldsymbol{\lambda}), \quad \Theta(\boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{\lambda}^T\mathbf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathbf{d},$$

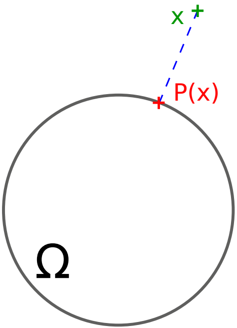
kde

$$\mathbf{F} := \tilde{\mathbf{B}}\mathbf{K}^{-1}\tilde{\mathbf{B}}^T, \quad \mathbf{d} := \tilde{\mathbf{B}}\mathbf{K}^{-1}\mathbf{f} - \tilde{\mathbf{c}}.$$

QPQC

$$\Omega := \{\mathbf{x} \in \mathbb{R}^n : \sqrt{x_{2i-1}^2 + x_{2i}^2} \leq r_i, \text{ for all } i = 1, \dots, m\}.$$

$$P_\Omega(\mathbf{x}) := \begin{bmatrix} \frac{r_1}{\|[x_1, x_2]\|}[x_1, x_2]^T \\ \vdots \\ \frac{r_i}{\|[x_{2i-1}, x_{2i}]\|}[x_{2i-1}, x_{2i}]^T \\ \vdots \\ \frac{r_m}{\|[x_{2m-1}, x_{2m}]\|}[x_{2m-1}, x_{2m}]^T \end{bmatrix}$$



Modified proportioning with gradient projections (MPGP)

Algoritmus 1 MPGP

```
Choose $x_0 \in \Omega, \alpha \in (0, 2\|A\|^{-1}), \delta \in (0, 1/2\rangle$
$k := 0$
while $\|\tilde{g}_k\| \geq \epsilon\|b\|$ do
    if $2\delta g_k^T g_k^P \leq \|\varphi(x_k)\|^2$ then
        CG step or CG halfstep.
        make CG step to solve problem on free set.
        if this step means leaving $\Omega$, do only a half-step and restart CG.
        $k := k + 1$
    else
        Projection step.
        $x_{k+1} := P(x_k - \alpha g_k)$
        restart CG
        $k := k + 1$
    end if
end while
```

Spectral projected gradient method (SPG)

Algoritmus 2 SGP

Choose $\boldsymbol{x}_0 \in \Omega,\ 0 < \alpha_{min} \leq \alpha_0 \leq \alpha_{max},\ 0 < \sigma_1 < \sigma_2 < 1,\ \gamma \in (0,1)$

$k := 0$

while $\|P(\boldsymbol{x}_k - \alpha_k \boldsymbol{g}_k) - \boldsymbol{x}_k\| > \epsilon$ **do**

  $\boldsymbol{d}_k := P(\boldsymbol{x}_k - \alpha_k \boldsymbol{g}_k) - \boldsymbol{x}_k$

  Find $\lambda \in \langle \sigma_1, \sigma_2 \rangle$ such that

$$f(\boldsymbol{x}_k + \lambda \boldsymbol{d}_k) \leq f(\boldsymbol{x}_k) + \gamma \lambda \langle \boldsymbol{d}_k, \boldsymbol{g}_k \rangle$$

  $\boldsymbol{x}_{k+1} := \boldsymbol{x}_k + \lambda \boldsymbol{d}_k$

  $\boldsymbol{s}_k := \boldsymbol{x}_{k+1} - \boldsymbol{x}_k$

  $\boldsymbol{y}_k := \boldsymbol{g}_{k+1} - \boldsymbol{g}_k$

  $\alpha_{k+1} := \min\{\alpha_{max}, \max\{\alpha_{min}, \frac{\langle \boldsymbol{s}_k, \boldsymbol{s}_k \rangle}{\langle \boldsymbol{y}_k, \boldsymbol{s}_k \rangle}\}\}$

  $k := k + 1$

end while

Modified proportioning with Barzilai-Borwein gradient projections (MPGP-BB)

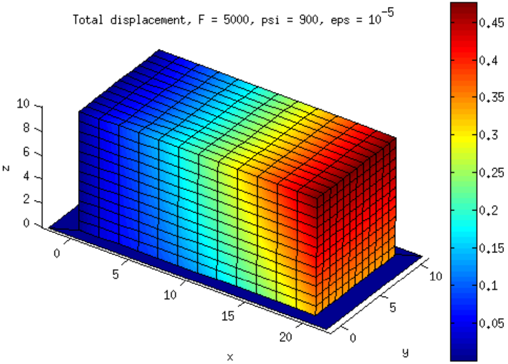
- měnit délku projektovaného gradientu dle SPG *bez* dodatečného GLL (uvolnění vazby, $f(\mathbf{x})$)

Algoritmus 3 MPGP-BB

Choose $\boldsymbol{x}_0 \in \Omega, \alpha \in (0, 2\|A\|^{-1}), \delta \in (0, 1/2\rangle$
$\alpha_{bb} := \alpha$
$k := 0$
while $\|\tilde{\boldsymbol{g}}_k\| \geq \epsilon\|b\|$ **do**
  if $2\delta \boldsymbol{g}_k^T \boldsymbol{g}_k^P \leq \|\varphi(\boldsymbol{x}_k)\|^2$ **then**
    CG step or CG halfstep.
    make CG step to solve problem on free set.
    if this step means leaving Ω, do only a half-step and restart CG.
    $k := k + 1$
  else
    Projection step.
    $\boldsymbol{x}_{k+1} := P(\boldsymbol{x}^k - \alpha_{bb}\boldsymbol{g}_k)$
    $\boldsymbol{s} := \boldsymbol{x}_{k+1} - \boldsymbol{x}_k$
    $\alpha_{bb} := \boldsymbol{s}^T\boldsymbol{s}/\boldsymbol{s}^T\boldsymbol{A}\boldsymbol{s}$
    restart CG
    $k := k + 1$
  end if
end while

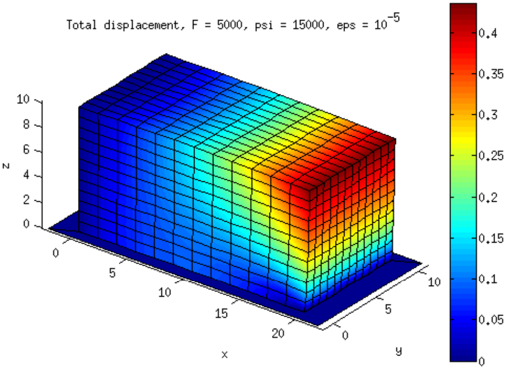
Numerické testy

Pro implementaci využit Matlab + MatSOL.
Konkrétní hodnoty: ocel, $\psi = 900$, $F = 5000$, $\epsilon = 10^{-5}$
primární proměnné: 6591, duální proměnné: 507
aktivní vazby: 93/169 Q, 39/169 L



Numerické testy

Konkrétní hodnoty: ocel, $\psi = 15000, F = 5000, \epsilon = 10^{-5}$
primární proměnné: 6591, duální proměnné: 507
aktivní vazby: 0/169 Q, 35/169 L



Numerické testy

F = 5000, ψ = 900, $\epsilon = 10^{-4}$												
N	**primal**	**dual**	**SPG**	**MPGP**				**MPGP-BB**				**active**
			it	it	cg	half	proj	it	cg	half	proj	Q,L
4	375	75	36	5176	0	1	5175	41	0	1	40	11/25, 10/25
6	1029	147	45	2746	0	1	2745	57	0	1	56	27/49, 21/49
8	2187	243	27	1236	0	1	1235	51	0	1	50	44/81, 27/81
10	3993	363	33	661	0	1	660	40	0	1	39	76/121, 33/121

F = 5000, ψ = 5000, $\epsilon = 10^{-4}$												
N	**primal**	**dual**	**SPG**	**MPGP**				**MPGP-BB**				**active**
			it	it	cg	half	proj	it	cg	half	proj	Q,L
4	375	75	1128	3191	177	15	2999	216	15	25	176	3/25, 10/25
6	1029	147	479	2005	25	18	1962	139	8	53	78	5/49, 14/49
8	2187	243	341	1860	5	22	1833	125	1	45	79	6/81, 23/81
10	3993	363	199	1078	2	30	1046	103	2	51	50	5/121, 31/121

F = 5000, ψ = 15000, $\epsilon = 10^{-4}$												
N	**primal**	**dual**	**SPG**	**MPGP**				**MPGP-BB**				**active**
			it	it	cg	half	proj	it	cg	half	proj	Q,L
4	375	75	1566	43	33	9	1	43	33	9	1	0/25, 10/25
6	1029	147	923	48	29	18	1	48	29	18	1	0/49, 14/49
8	2187	243	588	53	24	28	1	53	24	28	1	0/81, 18/81
10	3993	363	1020	101	40	46	15	73	27	40	6	0/121, 27/121

Několik poznámek ke konvergenci

- **MPGP** (Dostál, Schöberl, Kozubek) projekce s konstantní délkou kroku $\alpha \in (0, 2/\|A\|)$ zaručuje pokles cenové funkce v každé iteraci

$$\mathbf{x}_{k+1} := P(\mathbf{x}_k - \alpha \mathbf{g}_k)$$
$$f(\mathbf{x}_{k+1}) - f(\bar{\mathbf{x}}) \leq (1 - \alpha \lambda^{\mathbf{A}}_{\max})(f(\mathbf{x}_k) - f(\bar{\mathbf{x}}))$$

- **SPG** (Martínez, Birgin, Raydan) konvergence je zaručena splněním Armijo podmínky v každé iteraci

$$\mathbf{d}_k := P(\mathbf{x}_k - \alpha_k \mathbf{g}_k) - \mathbf{x}_k$$
$$\text{find} \quad \lambda : \quad f(\mathbf{x}_k + \lambda \mathbf{d}_k) \leq f(\mathbf{x}_k) + \gamma \lambda \langle \mathbf{d}_k, \mathbf{g}_k \rangle$$
$$\mathbf{x}_{k+1} := \mathbf{x}_k + \lambda \mathbf{d}_k$$

Několik poznámek ke konvergenci

- **MPGP-BB**
  - délka kroku není konstatní a numerické testy naznačují, že pokles cenové funkce není monotónní (BB není monotónní ani v neprojektované verzi)
  - původní Raydanův důkaz neprojektovaného BB je založen na konvergenci souřadnic chyby $\mathbf{x}_k - \hat{\mathbf{x}}$ v bázi vlastních vektorů matice $\mathbf{A}$
  - Armijo podmínka není splněna v každé iteraci

Několik poznámek ke konvergenci

Pro QP na konvexních množinách se mi *zatím* podařilo odvodit

$$f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) + \gamma_k \langle \mathbf{x}_{k+1} - \mathbf{x}_k, \mathbf{g}_k \rangle$$

kde

$$\gamma_k := \left(1 - \frac{\alpha_k}{2\alpha_{k+1}}\right) .$$

Děkuji za pozornost

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