

## Errata for “Nonlinear Programming: Concepts, Algorithms and Applications to Chemical Engineering”

- p. 28, line 11: change “ $f(x) = x^4 \cos(1/x)$ ” to “ $f(x) = x^4(2 + \cos(1/x))$ ”
- pp. 27-30, various places: change “ $p^T \nabla^2 f(x^* + \tau p)^T p < 0$ ” to “ $p^T \nabla^2 f(x^* + \tau p) p < 0$ ” and “ $p^T \nabla^2 f(x^* + tp)^T p < 0$ ” to “ $p^T \nabla^2 f(x^* + tp) p < 0$ ”
- p. 29, line 26: change “ $\frac{t^2}{2} p^T \nabla^2 f(x + \tau p)^T p < 0$ ” to “ $\frac{t^2}{2} p^T \nabla^2 f(x^* + \tau p) p < 0$ ”
- p. 35, lines 22, 24: change “ $\nabla^2 f(x^k + t(x^k - x^*))$ ” to “ $\nabla^2 f(x^k + t(x^* - x^k))$ ”
- p. 45, change Equation (3.23) to:  $u^k = \frac{B^k s^k}{[(s^k)^T B^k s^k]^{1/2}}$ , and  $v^k = \frac{y^k}{((y^k)^T s^k)^{1/2}}$ .
- p. 48, line 13: change “if  $(1 - \eta) > \zeta$ ” to “if  $(1 - \eta) < \zeta$ ”
- p. 49, line -3: change “ $\kappa(B^k)$ ” to “ $\kappa(B^k)$ ”
- p. 64, last three lines: change “ $g$ ” to “ $g_i$ ”
- p. 71, First line of Equation (4.12) should read:  $p^T \nabla_{xx} L(x^*, u^*, v^*) p \geq 0$ ,
- p. 72, Equation (4.24) should read: 
$$= \begin{bmatrix} 2 + \frac{1}{(x_1^*)^2} & 1 - u^* \\ 1 - u^* & 3 + \frac{1}{(x_2^*)^2} \end{bmatrix} = \begin{bmatrix} 2.5 & 0.068 \\ 0.068 & 3.125 \end{bmatrix}$$
- p. 78, line 9: change to “ $h_i(x^k) = t^k \nabla h_i(x^*)^T d = 0$ ”
- p. 80, line 23: change to “We now assume that  $d^T \nabla_{xx} L(x^*, u^*, v^*) d < 0$ ”
- p. 83, Equation (4.66) should read: 
$$= \begin{bmatrix} 2 + \frac{1}{(x_1^*)^2} & 1 - u^* \\ 1 - u^* & 3 + \frac{1}{(x_2^*)^2} \end{bmatrix} = \begin{bmatrix} 2.3093 & 0.4315 \\ 0.4315 & 3.2021 \end{bmatrix}$$
- p. 83, last line, change to  $(Q^N)^T \nabla_{xx} L(x^*, u^*, v^*) Q^N = 2.4272$
- p. 86, in (4.75), change “min” to “max”
- p. 92, in (5.2), change “ $\nabla h(x^*)^T v^*$ ” to “ $\nabla h(x^*) v^*$ .”
- p. 93, line 18: change  $\|\nabla L(x^k, v^k)\| > \epsilon_2$  to  $\max(\|\nabla L(x^k, v^k)\|, \|h(x^k)\|) > \epsilon_2$ .
- p. 93, line 19: change “Evaluate  $\nabla f(x^k)$ ” to “Evaluate  $h(x^k), \nabla f(x^k)$ ”
- pp. 104-109: change  $d_x$  to  $d_x^k$  in (5.41)-(5.43) and (5.51), (5.53), (5.54).
- p. 108: change “ $x^{k+2}$ ” to “ $x^k + d_x^k + d_x^{k+1}$ ” in (5.52).
- p. 110, line 16: change “trail point” to “trial point”
- p. 116, in (5.70) and after (5.72), change “ $(Z^k)^T f(x^k)$ ” to “ $(Z^k)^T \nabla f(x^k)$ ”
- p. 118, line 19: change to “The Hessian  $W(x, v)$  or its approximation”
- p. 129, change  $\bar{d}$  to  $\bar{d}_x$  in (5.111).
- p. 140, line 19; p. 178, line 25: change  $[0, 0.1]$  to  $[0, 0.1, 0, 0]^T$

- p. 140, line 30; p. 178, line 25: change  $[0, 0]$  to  $[0, 0, 0, 0]^T$
- p. 158, second part of (6.65) should read “ $\liminf_{k \rightarrow \infty} \|\nabla \varphi_\mu(x^k) + \nabla c(x^k)v^k\| = 0$ .”
- p. 160, line 6: change to “ $\varphi_\mu(x)$  is bounded below and  $x$  is bounded above and below.”
- p. 160, line 14: change to “boundedness assumption for  $\varphi_\mu$  and  $x$ ,”
- p. 166, Equation (6.81) should read:  $\epsilon^k = \min[\|z^k - \mathcal{P}(z^k - \nabla f(z^k))\|, \min_i(z_{U,(i)} - z_{L,(i)})/2]$
- p. 189, lines 27-28, change to:

$$g(x^0) = \nabla f(x^0) + \frac{1}{2} \Delta(\epsilon + 1/\epsilon)[1 \ 1]^T = (2\epsilon\beta + \Delta(\epsilon + 1/\epsilon)/2)[1 \ 1]^T$$

where second term is the truncation error from the perturbation  $\Delta^{1/2}$ ...

- p. 216, line 16: replace “(8.5g)” by “(8.5d)-(8.5g)”
- p. 222: in (8.8) change  $[\frac{\partial f}{\partial z} \lambda - \frac{d\lambda}{dt} + \frac{\partial g_E}{\partial z} \nu_E + \frac{\partial g_I}{\partial z} \nu_I]^T \delta z(t)$  to  $[\frac{\partial f}{\partial z} \lambda + \frac{d\lambda}{dt} + \frac{\partial g_E}{\partial z} \nu_E + \frac{\partial g_I}{\partial z} \nu_I]^T \delta z(t)$
- p. 225, line 1: change  $k = k_{20}/k_{10}$  to  $k = k_{20}/(k_{10}^\beta)$
- pp. 235-236: replace (8.39h), (8.40e) and (8.41e) by  $1 = \sum_{i=1}^{NC} x_i$
- p. 236, line 23: replace  $\sum_{i=1}^{NC} (K_i(T, P) - 1) \frac{dx_i}{dt} = 0$  by  $\sum_{i=1}^{NC} \frac{dx_i}{dt} = 0$ .
- p. 236, line 25, p. 237 (8.41f): replace by  $\sum_{i=1}^{NC} [F(t)(z_i(t) - x_i(t)) - V(t)(y_i(t) - x_i(t))]/M(t) = 0$
- p. 238, change second line of (8.44) to  
“ $= \lambda_1 z_2(t) + \lambda_2 u(t) + 1 + \nu_I u(t) + \nu_U(u(t) - u_U) + \nu_L(u_L - u(t))$ ”
- p. 242, change line 4 to:  $-k_3 b(t_f) = H(0) = J(0)u(0) - \lambda_2 k_3 b(0) = J(0)u(0) < 0$
- p. 243, line 15: change “for  $k_1 = 1$ ,” to “for  $a_0 = 1, k_1 = 1$ ,”
- p. 261: line 19: change equation  $\nabla_p \Psi^T = \frac{\partial \Psi^T}{\partial z} S(t_f) + \frac{\partial \psi^T}{\partial p}$   
to  $\nabla_p \Psi = S(t_f)^T \frac{\partial \Psi}{\partial z} + R(t_f)^T \frac{\partial \Psi}{\partial y} + \frac{\partial \Psi}{\partial p}$
- p. 263: in (9.26) change  $[\frac{\partial f}{\partial z} \lambda - \frac{d\lambda}{dt} + \frac{\partial g}{\partial z} \nu]^T \delta z(t)$  to  $[\frac{\partial f}{\partial z} \lambda + \frac{d\lambda}{dt} + \frac{\partial g}{\partial z} \nu]^T \delta z(t)$
- p. 268: Modify equation (9.42) and above “rewritten as:

$$\frac{d\psi}{dp^l} = \frac{\partial \psi}{\partial p^l} + \int_{t_{l-1}}^{t_l} \left[ \frac{\partial f}{\partial p^l} \lambda + \frac{\partial g}{\partial p^l} \nu \right] dt."$$

to: “rewritten for the objective function  $\varphi$  as:

$$\frac{d\varphi}{dp^l} = \frac{\partial \varphi}{\partial p^l} + \int_{t_{l-1}}^{t_l} \left[ \frac{\partial f}{\partial p^l} \lambda + \frac{\partial g}{\partial p^l} \nu \right] dt."$$

- p. 268: Add  $h_l \geq 0$  to end of (9.43e)

- p. 270: above (9.47), change: “The corresponding integrals for the decision variables, are given by” to “The corresponding integrals for the derivatives of the objective function ( $\varphi = -b(N_T)$ ), with respect to decision variables, are given by”
- From last paragraph on p. 289 to (10.6), change to: “Equivalently, the *time derivative* of the state in element  $i$  can be represented as a Lagrange polynomial with  $K$  interpolation points, i.e.,

$$\frac{dz^K(t)}{d\tau} = \sum_{j=1}^K \bar{\ell}_j(\tau) \dot{z}_{ij},$$

where  $\dot{z}_{ij}$  represents  $\frac{dz^K(t_{ij})}{d\tau}$  and  $\bar{\ell}_j(\tau) = \prod_{k=1, k \neq j}^K \frac{(\tau - \tau_k)}{(\tau_j - \tau_k)}$ . For element  $i$  this leads to the *Runge-Kutta* basis representation for the differential state:

$$z^K(t) = z_{i-1} + h_i \sum_{j=1}^K \Omega_j(\tau) \dot{z}_{ij} \quad (10.5)$$

where  $z_{i-1}$  is a coefficient that represents the differential state at the beginning of element  $i$  and  $\Omega_j(\tau)$  is a polynomial of order  $K$ , satisfying

$$\Omega_j(\tau) = \int_0^\tau \bar{\ell}_j(\tau') d\tau', \quad t \in [t_{i-1}, t_i], \quad \tau \in [0, 1].$$

To determine the polynomial coefficients that approximate the solution of the DAE, we substitute the polynomial into (10.2) and enforce the resulting algebraic equations at the interpolation points  $\tau_k$ . This leads to the following *collocation equations*:

$$\frac{dz^K(t_{ik})}{dt} = f(z^K(t_{ik}), t_{ik}), \quad k = 1, \dots, K, \quad (10.6)$$

- p. 291-292, change (10.13) to  $P_K^{(\alpha, \beta)} = \sum_{j=0}^K (\tau - 1)^j \gamma_j$  with  $\gamma_j = \frac{(\alpha + K)! (\alpha + \beta + K + j)!}{(\alpha + j)! (\alpha + \beta + K)! (K - j)! j!}$ ,  $j = 0, \dots, K$ .
- p. 296, lines 11, 12: change “ $T(t)$ ” to “ $T_i(t)$ ”
- p. 296, line -4: change “is obtained automatically, as algebraic variables are implicit functions of continuous differential variables.” to “can be determined directly from the continuous differential variables at  $t_i$ .”
- p. 297, lines 6,7 and in (10.21b): change “ $t_{nc}$ ” to “ $t_{i,nc}$ ”
- p. 342, change (11.41a), (11.41b) from:

$$\begin{aligned} \bar{G}_i^{ig}(T, P) + RT \ln(f_i^L) + \left\{ \sum_{i=1}^{NC} (l_i \frac{\partial \bar{G}_i^L}{\partial l_i} + v_i \frac{\partial \bar{G}_i^V}{\partial l_i}) \right\} - \alpha_L - \gamma_i &= 0 \\ \bar{G}_i^{ig}(T, P) + RT \ln(f_i^V) + \left\{ \sum_{i=1}^{NC} (l_i \frac{\partial \bar{G}_i^L}{\partial v_i} + v_i \frac{\partial \bar{G}_i^V}{\partial v_i}) \right\} - \alpha_V - \gamma_i &= 0 \end{aligned}$$

to

$$\begin{aligned} \bar{G}_i^{ig}(T, P) + RT \ln(f_i^L) + \left\{ \sum_{j=1}^{NC} (l_j \frac{\partial \bar{G}_j^L}{\partial l_i} + v_j \frac{\partial \bar{G}_j^V}{\partial l_i}) \right\} - \alpha_L - \gamma_i &= 0 \\ \bar{G}_i^{ig}(T, P) + RT \ln(f_i^V) + \left\{ \sum_{j=1}^{NC} (l_j \frac{\partial \bar{G}_j^L}{\partial v_i} + v_j \frac{\partial \bar{G}_j^V}{\partial v_i}) \right\} - \alpha_V - \gamma_i &= 0 \end{aligned}$$

- p. 342, in (11.42b) change  $\beta = 1 - s_L + s_V$  to  $-s_L \leq \beta - 1 \leq s_V$ .

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