

NOMENCLATURE

a	coefficient in quadratic function
a_i	lower bound on constraint function
a_{pi}	crude oil yield
A	annual revenue
A	area
A_i^l	lower bound on analysis for component i
A_i^u	upper bound on analysis for component i
A	coefficient matrix in linear constraint
A	Jacobian matrix of constraints
\bar{A}	adjoint matrix of A
AL	augmented Lagrangian function
b	coefficient in quadratic function
b_i	i th parameter estimate
b_i	upper bound on constraint function
b_{ij}	coefficients in quadratic function
\mathbf{b}	vector of coefficients in equality constraints
B	barrier function
\mathbf{B}	basis matrix
\mathbf{B}	approximation to the Hessian matrix used in sequential quadratic programming
c	coefficient in quadratic function
c	constant in rate of convergence
c_j	right-hand side, inequality constraint
\mathbf{c}	vector of cost coefficients
C	cost
C_B	base cost

$C_{j,k}$	completion time (see Example 16.2)
d_j	depreciation taken in year j
d_{ij}	coefficient in quadratic function
d^k	vector in BFGS method
\mathbf{d}_c	search vector
D	number of units produced in manufacturing
D	diameter
D_j	cumulative depreciation in year j
D_p	maximum demand
\mathbf{D}	diagonal matrix
dn_i	negative deviation variable
dp_i	positive deviation variable
e	measurement error
e_i	i th eigenvalue
E	error measure
E	annual expense
f	objective function
f_{low}	lowest estimated value of f
F	reduced objective function
F_i	future value or payment in year i
g_j	inequality constraint
$g(\alpha)$	line search objective function
\mathbf{g}	vector of inequality constraints
h	step size in discretization
h_j	equality constraint
\mathbf{h}	vector of equality constraints
\mathbf{H}	Hessian matrix
$\tilde{\mathbf{H}}$	modified Hessian matrix in Equation (6.16)
\mathbf{H}^k	approximation of \mathbf{H} at iteration k
\mathbf{H}^{-1}	inverse Hessian matrix
i	interest rate
I_x	cost index factor
\mathbf{I}	identity matrix
J	mathematical operator
\mathbf{J}	Jacobian matrix
k	iteration number
k_i	cost coefficients
\mathbf{l}	lower bound
L	Lagrangian
L_i, l_i	lower bound
\mathbf{L}	lower triangular matrix
m	slope
m	number of equality constraints
m	rank of matrix
m	number of control moves

m_e	number of independent equality constraints
m_i	number of independent inequality constraints
M	penalty coefficient (big M method)
M_i	i th minor of matrix
\mathbf{M}	matrix in MINLP
n	dimension of \mathbf{x}
n	number of time periods in investment project
n	number of data sets
$n1$	negative deviation variables
N	number of terms in Equation (16.1)
\mathbf{N}	matrix involving nonbasic variables
p	number of variables
p	total number of constraints
p	order of convergence
p	prediction horizon
$p1$	positive deviation variables
$p^{(i)}$	job scheduling index
P	present value
P,p	penalty function
\mathbf{P}	job scheduling vector
q	weighting factor in model predictive control
Q	production level
\mathbf{Q}	weighting matrix in quadratic programming
\mathbf{Q}	positive-definite matrix
r	number of inequality constraints
r	repayment multiplier
r	line search objective
$r(k)$	setpoint
r	penalty function weighting coefficient
s_i	slack or surplus variable
s_i	component of a search direction
\mathbf{s}	search direction
S	size parameter
S_i	supply limit
S_i	step response coefficient
S_v	salvage value
S_c^{Ki}	relative sensitivity of cost to coefficient K_i
t	time
T	simulated annealing variable
$t_{j,k}$	processing time (see Example 16.2)
\mathbf{u}	vector of Lagrange multipliers
\mathbf{u}	upper bound
U_i, u_i	upper bound
$u(k)$	manipulated variable
v_i	value coefficient

v_i	i th eigenvector
v_i	vector defined in necessary conditions
V_j	book value in year j
\bar{V}	optimal objective value
\mathbf{V}	eigenvector matrix
\mathbf{V}	variance–covariance matrix
w	factor in Equation (5.18)
w_i	weighting factor in Equation (16.2)
w_1	positive weight in penalty function
x_{ij}	variable in assignment problem
\mathbf{x}	vector of n variables
\mathbf{x}	model input vector
\mathbf{x}_B	vector of basic variables
\mathbf{x}_D	dependent variables
\mathbf{x}_I	independent variables
\mathbf{x}^k	optimization variable at iteration k
\mathbf{x}_N	vector of nonbasic variables
\mathbf{x}^p	reference point
\mathbf{x}_T	tear variables
\mathbf{x}^*	optimal value of \mathbf{x}
$\tilde{\mathbf{x}}^*$	approximation to \mathbf{x}^*
\mathbf{x}	data matrix
X_{ij}	binary variable in objective function
y	model output
Y	optimization variable
Y_m	measured variable value
Y	operating hours per year
Y_j	observed data point
\mathbf{y}	integer variable vector
z	distance variable
z	MINLP objective function term

GREEK SYMBOLS

α	distance moved along a search vector (step length)
β	positive weighting factor
β_j	model parameter
$\hat{\beta}_j$	estimated model parameter
β^k	step size adjustment in conjugate gradient method
γ	positive weighting factor
δ	bound on step size
δ	parameter in convexity definition
∇	gradient operator (“del”)

Δ	difference in general
Δ	determinant
Δt	discretization in time for model predictive control
Δu	change in manipulated variable
$\Delta \mathbf{x}^k$	$\mathbf{x}^{k+1} - \mathbf{x}^k$
Δ_i	determinant of i th principal minor
ε	roundoff error
ε_i	convergence (termination) criterion
ε_j	random error between j th data point and model prediction
λ	vector of Lagrange multipliers
θ	angle between two vectors
ρ	a scalar between 0 and 1
$\tau_{j,k}$	scheduling variable (see Example 16.2)
ϕ_k	vector of tear variables in flowsheet optimization

SUPERSCRIPTS

k	stage in search
T	transpose
o	at optimal solution
opt	optimum
'	first derivative
*	optimum

NAME INDEX

- Abadie, J., 306, 328
 Abel, O., 514
 Adjiman, C. S., 373, 412, 496, 513
 Agnew, J. B., 449, 458
 Aldrich, C., 413
 Alkaya, D., 548
 Amundson, N. R., 142, 600
 Anderson, J. L., 459
 Androulakis, I. A., 373, 412, 496, 498–500, 513
 Angeline, P. J., 413
 Aragon, C. R., 399, 412
 Arlt, W., 452, 453, 458
 Armijo, L., 205, 210
 Ashdee, B. T., 478
 Athier, G., 419, 438
 Avriel, M., 142, 186, 210, 395, 411
 Azzaro-Pantel, C., 413

 Backx, T., 575, 579
 Badgwell, T. A., 508, 513, 568, 581
 Baile, R. C., 329, 604, 610, 629
 Baker, T. E., 306, 328, 553, 554, 565, 579, 580
 Balakrishna, A., 548
 Balakrishna, S., 514
 Bar-Kana, I., 84, 104, 629
 Barnes, J. W., 393, 395, 411, 412
 Barsky, B., 116, 142
 Bartela, R., 116, 142
 Bates, D. M., 62, 73
 Baudet, P., 413
 Bauer, M. H., 443, 446, 458
 Baumol, W. J., 20, 27
 Bazarra, M. S., 142, 159, 176
 Beatty, J., 116, 142
 Becker, H. A., 176, 179
 Beightler, C. S., 177
 Bejan, A., 478
 Bendor, E. A., 73
 Bequette, B. W., 73, 459, 501, 503–505, 508, 513
 Berna, T. J., 319, 328
 Bernal-Haro, L., 413
 Beveridge, G. S. G., 6, 27, 138, 142, 176
 Bhaskar, V., 104

 Bhatia, T. K., 329
 Biegler, L. T., 329, 372, 443, 458, 459, 514, 529, 542–548, 577, 581
 Biles, W. E., 66, 73
 Bird, R. B., 51, 69, 73
 Bischof, C., 546
 Bischoff, K. B., 481, 513
 Bixby, R. E., 238, 253
 Black, J. H., 610, 617, 629
 Blank, L. T., 105
 Boddington, C. E., 581
 Boggs, P. T., 211
 Bonvin, D., 514
 Bordons, C., 568, 580
 Borwein, J., 142
 Bosgra, O., 575, 579
 Boston, J. F., 548
 Bowman, M. S., 105
 Box, G. E. P., 48, 60, 62, 66, 73
 Brent, R. P., 177, 211
 Brigham, E. F., 617, 618, 628
 Brinn, M. S., 423, 427, 439
 Briones, V., 419, 439
 Britt, H. I., 548
 Brooke, A., 323, 328
 Brooks, S. A., 329
 Brown, G. G., 290, 328
 Broyden, C. G., 208, 210, 211
 Brummerstedt, E. F., 88, 104
 Brunger, A. T., 496, 513
 Bryant, G. F., 553, 554, 565, 579
 Bunch, J. R., 598, 600
 Bunch, P. R., 561, 580
 Burwick, C. W., 492, 513
 Byrd, R. H., 211

 Caballero, J. A., 373
 Camacho, E. F., 568, 580
 Campbell, H. G., 600
 Canada, J. R., 105
 Carle, A., 546
 Carpentier, J., 306, 328
 Carroll, J. A., 478
 Cerda, J., 373

- Chaudhuri, P. D., 439
 Chen, H. S., 543, 546, 548
 Cheng, Y., 576, 581
 Choi, H., 413
 Churchill, S. W., 73
 Cichelli, M. T., 423, 427, 439
 Ciric, A. R., 439
 Colmenares, T. R., 439
 Converse, A. O., 488–490, 513
 Cook, L. N., 176, 179
 Cooley, B., 581
 Cooper, L., 177
 Corliss, G. F., 546, 547
 Cornellisen, R. L., 439
 Corripio, A. B., 609, 629
 Coville, A. R., 492, 513
 Crainic, T. G., 390, 411
 Cramer, S. M., 459
 Crellin, R., 253
 Crowder, H. P., 373
 Crowe, C. M., 576, 580, 581
 Cugini, J. C., 254
 Currie, J. C., 478
 Curtis, A. R., 535, 547

 Daichendt, M. M., 439, 548
 Dallwig, S., 412
 Daniel, J. W., 601
 Dantzig, G. B., 223, 227, 230, 232, 239, 253
 Darst, R. B., 253
 Davidson, H., 577, 580
 Davis, J. F., 554, 565, 578, 579, 581
 Davis, M. E., 73
 de Gouvêa, M. T., 329
 Deb, K., 413
 Dell, R. F., 290, 328
 Dembo, R. S., 195, 210
 Demenech, S., 413
 Demmel, J. W., 601
 Denn, M. M., 73
 Dennis, J. E., 155, 161, 176, 187, 203, 205, 208, 210
 Dennis, J. E., Jr., 329
 Detiz, D., 39, 73
 Devanathan, S., 576, 581
 DiBella, C. W., 328, 343
 Diwekar, U. M., 439, 548
 Dixon, L. C. W., 183, 210
 Domenech, S., 399, 400, 411
 Dongarra, J. J., 598, 600
 Doty, D. R., 478
 Douglas, J. M., 508, 510, 511, 513
 Douglas, P. L., 176, 179
 Drain, D., 63, 73
 Draper, N. R., 60, 66, 73

 Dreisbach, D., 452, 458
 Drud, A., 321, 328
 Duennebier, G., 458
 Duff, I. S., 526, 547
 Duong, D. D., 74
 Duran, M. A., 369, 371, 373, 439
 Duvall, P. M., 329

 Edgar, T. F., 62, 73, 354, 373, 508, 513, 514, 566, 567, 570, 577, 578, 580, 581
 Eduljee, H. E., 454, 458
 Edwards, K., 514
 Eisenstat, S. C., 195, 210
 El-Halwagi, M., 458
 Engell, S., 413, 561, 581
 Erisman, A. M., 526, 547
 Esplugas, S., 439
 Esposito, W. R., 413
 Espura, A., 559, 580
 Evans, B., 543, 547
 Eykhoff, P., 38, 73

 Fabbri, G., 439
 Fan, L. T., 74
 Fan, Y. S., 328
 Feinberg, M., 514
 Ferguson, J. E., 419, 422, 439
 Fiacco, A. V., 525, 547
 Finlayson, B., 503, 513
 Fletcher, R., 194, 195, 208, 210
 Floquet, R., 399, 400, 411, 419, 438
 Floudas, C. A., 363, 369, 371, 373, 388, 398, 412, 413, 439, 458, 459, 496, 498, 513, 514, 548
 Fogel, D. B., 402, 412, 413
 Fogler, H. S., 481, 513
 Forbes, F., 576, 580
 Forrest, J. J., 238, 253
 Fourer, R. D., 245, 253, 323, 328
 Fox, R. L., 139, 142, 175, 176
 Fragar, E. S., 443, 458, 508, 511–513
 Freeman, M., 413
 Frey, Th., 443, 458, 466
 Friedly, J. C., 73
 Frieze, T., 413
 Froment, G. F., 481, 513
 Fylstra, D. L., 322, 328, 360, 373

 Galli, M. R., 373
 Gaminibandara, K., 446, 447, 458
 Garcia, C. E., 568, 569, 580, 581
 Garrad, A., 413
 Garrett, D. E., 94, 104, 604, 605, 610, 618
 Gass, S. I., 253
 Gay, D. M., 323, 328

- Gebhart, B., 54, 73
 Geddes, D., 514
 Gelb, A., 577, 580
 Geoffrion, A. M., 370, 373
 Gill, P. E., 195, 210, 253, 517, 547
 Gilliland, E. R., 140, 142
 Glanz, S., 448, 458
 Glover, F. A., 252, 253, 392, 393, 395, 397, 402, 408, 411, 412
 Gmehling, T., 452, 453, 458
 Goldfarb, D., 208, 210, 238, 253
 Golub, G. H., 584, 596, 600
 Gooding, W. B., 581
 Gordon, S. R., 100, 104
 Graves, D. B., 501, 502, 513
 Greeff, D. J., 413
 Green, D. W., 354, 373, 533, 535, 547, 604, 618
 Griest, W. H., 618, 626
 Griewank, A., 546, 547
 Gross, B., 413
 Grossmann, I. W., 369, 371–374, 413, 419, 439, 529, 542, 546–548, 556, 558, 580
 Guez, A., 84, 104, 629
 Gunderson, T., 519, 547
 Guntern, C., 514
 Gupta, S. K., 104, 514

 Hale, J. C., 554, 565, 579, 581
 Hanagandi, V., 413
 Happell, J., 88, 89, 104, 142, 148
 Harding, S. T., 459
 Harjunkski, I., 374
 Harriott, P., 439, 465, 478
 Hartland, S., 449, 458
 Haupt, R. L., 413
 Heinemann, R. F., 478
 Helbig, A., 514
 Hendon, S. R., 516, 547
 Henson, M. A., 577, 578, 580
 Hestenes, M. R., 211
 Hext, G. R., 185, 211
 Hildebrandt, D., 514
 Hill, J. W., 60, 73
 Hillier, F., 27
 Himmelblau, D. M., 530, 547
 Himsworth, F. R., 185, 211
 Hiriart-Urruty, J. D., 401, 412
 Hiss, G. G., 439
 Hochberg, A. K., 500, 513
 Holland, C. D., 443, 447, 458
 Holland, J. H., 401, 412
 Hooker, J., 372, 373
 Horne, R. N., 478, 479
 Horoka, F., 452, 458
 Hrymak, A. N., 567, 580

 Hubele, N. F., 74
 Hughes, R. R., 543, 547
 Huh, D., 479
 Hungerbühler, K., 514
 Hunter, J. S., 73
 Hunter, W. G., 60, 73
 Hurvich, C., 84, 104

 Ierapetritou, M. G., 496, 498–500, 513
 Ilias, S., 176, 179
 Iribarren, O. A., 540, 547

 Jaakola, T., 328, 330
 Jackson, J. E., 55, 73
 Jackson, P. J., 449, 458
 James, L., 183, 210
 Jegede, F. O., 419, 439
 Jelens, F. C., 610, 617, 629
 Jensen, K. F., 501, 502, 513
 Jeter, M. W., 142
 Jillier, F. S., 354, 373
 Johnson, E. L., 373
 Johnson, J. D., 253
 Johnston, D. S., 399, 412
 Jordan, D. G., 88, 89, 104, 142, 148
 Joulia, X., 545, 548
 Jung, J. H., 413

 Kamimura, R., 84, 104
 Kaplan, W., 142
 Karimi, I. A., 556, 558, 560–563, 580
 Karmarkar, N., 253
 Karr, C. L., 413
 Kearfott, R. B., 382, 412
 Keller, A. H., 514
 Kelley, C. T., 211
 Kennedy, C. J., 478
 Kernighan, B. W., 323, 328
 Kim, N., 298, 301, 329
 Kimpel, R. R., 328, 346
 Kinnear, K. E., Jr., 413
 Kisala, T. P., 548
 Klein, M., 328, 346
 Klepeis, J., 496, 498–500, 513
 Klingman, D., 252, 253
 Kluzik, H., 543, 547
 Ko, J. W., 413
 Koehret, B., 545, 548
 Kokossis, A. C., 373, 419, 439, 514, 548
 Kolari, M., 254
 Kondili, E., 581
 Koppel, L. B., 428, 429, 439
 Kravanja, Z., 373, 548
 Ku, H. M., 560–563, 580
 Kubera, T., 514

- Kuehn, D. R. D., 577, 580
 Kuri, C. J., 609, 629

 Laguna, M., 392, 393, 395, 397, 402, 408, 411, 412
 Lakshmanan, A., 329, 514
 Lang, Y. D., 543, 547, 548
 Lapidus, L., 74, 542, 547
 Laporte, G., 390, 411
 Lasdon, L., 298, 301, 306, 313, 320, 322, 328, 329, 360, 373, 553, 577, 580
 Latour, P. R., 454, 458
 Lee, B., 374
 Lee, C. H., 413
 Lee, E. S., 374
 Lee, I-B., 413
 Lee, J. H., 479, 569, 577, 580, 581
 Lee, S., 371, 373
 Lee, Y. G., 581
 LeGoff, P., 483
 Lemarichal, C., 401, 412
 Letterman, R. D., 467, 469, 478
 Levenberg, K., 202, 210
 Levenspiel, O., 418, 513
 Lewin, D. R., 74, 517, 547, 604, 629
 Lewis, A. S., 142
 Lewis, W. K., 140, 142
 Leyffer, S., 374
 Li, J., 211
 Lieberman, G. J., 27, 354, 373
 Liebman, J. F., 320, 328
 Liebman, M. J., 577, 580
 Lightfoot, E. N., 51, 69, 73
 Lim, H. C., 428, 429, 439
 Locatelli, M., 388, 412
 Locke, M. H., 319, 328
 Logsdon, J. S., 439, 459
 Löhl, T., 413
 Lowery, R. P., 516, 547
 Luenberger, D. G., 142, 176, 271, 279, 282, 286, 288, 291, 328, 330
 Luus, R., 328, 330, 514
 Luyben, W. L., 74
 Lyons, S. L., 478

 McAdams, W. H., 50, 140, 142, 427, 439
 McAvoy, T. J., 553, 580
 McCabe, W. L., 439, 465, 478
 Macchietto, S., 446, 458, 581
 McConville, B., 516, 547
 McCroskey, P. S., 581
 McDonald, C. M., 561, 580
 McGeoch, L. A., 399, 412
 MacGregor, J., 576, 580
 Mah, R. S. H., 540, 547, 576, 580, 581

 Mahalec, V., 543, 547
 Malone, M. F., 581
 Maloney, J. O., 604, 618
 Mangasarian, O. L., 207, 211
 Manousiouthakis, V., 413, 414, 458
 Maranas, G. D., 498, 499, 513
 Marguardt, W., 575, 579
 Marlin, T. E., 567, 576, 580
 Marquardt, W., 202, 211, 514
 Martin, G. D., 454, 458
 Martin, R. K., 223, 242, 243, 253
 Mata, J., 439
 Matias, T. R. S., 443, 458
 Mead, R., 186, 211
 Mecklenburgh, J. C., 449, 458
 Mellichamp, D. A., 62, 73, 566, 567, 570, 581
 Meloan, C. E., 442, 458
 Meyer, D., 584, 600
 Middleman, S., 500, 513
 Miller, D. L., 582
 Mims, C. A., 481, 513
 Missen, R. W., 481, 513
 Mistree, F., 177
 Mitchell, M., 413
 Mokashi, S. D., 373
 Moler, C. B., 598, 600
 Montagna, J. M., 540, 547
 Montgomery, D. C., 62, 73, 74
 Morari, M., 373, 556, 558, 568, 569, 580, 581
 Moré, J. J., 318, 320–322, 328
 Mujtaba, I. M., 446, 458
 Murase, A., 488–490, 513
 Murray, J. E., 354, 373
 Murray, W., 195, 210, 253, 517, 547
 Murtagh, B. A., 253, 310, 321, 328
 Murty, K. G., 253
 Muske, K., 577, 578, 580

 Narasimhan, S., 413
 Nash, S. G., 142, 155, 159, 176, 195, 211, 282, 292, 304, 305, 319, 328
 Natarajan, V., 459
 Nelder, J. A., 186, 211
 Nemethy, G., 496, 513
 Nemhauser, G. L., 353, 354, 356, 373
 Neumaier, A., 412
 Nikolaou, M., 413
 Nishikiori, N., 478
 Nocedal, J., 291, 292, 304, 328
 Noltie, C. B., 115, 142
 Novotrak, J. F., 478

 Odloak, D., 329
 Ogunnaike, T., 74

- Onken, U., 452, 453, 458
 Ostwald, P. F., 604, 629
 Otto, R. E., 329, 343

 Padberg, M. W., 373
 Palvia, S. C., 100, 104
 Pan, Y., 479
 Pantelides, C. C., 458, 581, 582
 Papageorgaki, S., 582
 Pardalos, P. M., 496, 513
 Parker, A. P., 543, 547
 Parker, R. G., 374
 Paules, G. E., 459
 Pekny, J. F., 560, 561, 565, 580–582
 Perkins, J. D., 516, 547, 582
 Perry, C., 253
 Peters, M. S., 27, 427, 439
 Pham, Q. T., 413
 Phillips, D. T., 177
 Phillips, N., 252, 253
 Phimister, J. R., 508, 511–513
 Pho, T. K., 542, 547
 Pibouleau, L., 399, 400, 411, 419, 438
 Pike, R. W., 559, 580
 Pilavachi, P. A., 439
 Pinter, J. D., 383, 412
 Pistikopoulos, E. N., 548
 Poje, J. B., 254
 Polley, G. T., 419, 439
 Pom, R., 374
 Pons, M., 545, 548
 Ponton, J. W., 508, 511–513
 Powell, M. J. D., 207, 211
 Prett, C. E., 568, 580
 Puigjaner, L., 559, 580

 Qin, J., 568, 581
 Quesada, I., 548

 Ragsdell, K. M., 28, 177, 211
 Rajagopalan, D., 580
 Rajesh, J. K., 514
 Ramagnoli, J. A., 18, 27
 Raman, R., 371, 373, 548
 Ramirez, W. F., 479, 526, 547
 Rangaiah, G. P., 514
 Rardin, R., 374
 Ravindran, A., 177, 211
 Rawlings, J. B., 577, 581
 Ray, A. K., 104, 514
 Ray, W. H., 74
 Redner, R. A., 478
 Reeves, C. M., 194, 195, 210
 Reeves, C. R., 401, 402, 412
 Reid, J. K., 526, 535, 547

 Reklaitis, G. V., 28, 177, 211, 318, 328, 459, 560, 565, 580, 582
 Reppich, M., 419, 439
 Rhinehart, R. R., 211
 Rice, R. G., 74
 Richalet, J., 568, 581
 Richard, L. A., 454, 458
 Riggs, J. B., 329
 Rinnooy Kan, A. H. G., 388, 389, 412
 Rippin, D. W. T., 554, 565, 579, 581
 Ritter, K., 207, 211
 Roberts, H. L., 488–490, 513
 Robertson, D., 577, 581
 Roenigk, K. F., 501, 513
 Rollins, D. K., 576, 578, 581
 Romagnoli, J. A., 575, 581
 Roosen, P., 413
 Rosen, J. B., 207, 211
 Rosenwald, G. W., 354, 373
 Rubin, E. S., 548
 Rudd, D. F., 28
 Rudof, R., 561, 581
 Runger, G. C., 74
 Rusnak, I., 84, 104, 629
 Rustem, B., 290, 328, 329

 Sama, D. A., 419, 422, 439
 Sanchez, M. C., 18, 27, 575, 581
 Sargent, R. W. H., 446, 447, 458, 581, 582
 Sarkar, S., 328
 Sarma, P. V. L. N., 318, 328
 Sauer, R. N., 492, 513
 Saunders, M. A., 253, 310, 321, 328
 Saville, B. A., 481, 513
 Schechter, R. S., 6, 27, 138, 142, 176
 Scheraga, H. A., 496, 513
 Schittkowski, K., 211
 Schlick, T., 496, 513
 Schmid, C., 443, 458, 529, 543, 544, 547
 Schmidt, L. D., 481, 513
 Schnabel, R. B., 155, 161, 176, 187, 203, 206, 208, 210, 211, 329
 Schrage, L., 254
 Schrijver, A., 254, 374
 Schulz, C., 413, 561, 581
 Schweiger, C. A., 514
 Schweyer, H. E., 439
 Seader, J. D., 74, 517, 547, 604, 629
 Seborg, D. E., 62, 73, 566, 567, 577, 578, 580, 581
 Seider, W. D., 74, 439, 517, 547, 604, 629
 Seinfeld, J. H., 74
 Sen, S., 413
 Setalvad, T., 501, 503–505, 508, 513
 Shaiwitz, J. A., 604, 610, 629

- Shaewitz, J., 329
 Shah, N., 582
 Shahbenderian, A. P., 59, 73
 Shalloway, D., 496, 513
 Shamir, R., 254
 Shanno, D. F., 208, 211
 Sherali, H. D., 142, 159, 176
 Shetly, C. M., 159, 176
 Shetty, C. M., 142
 Shobrys, D. E., 582
 Shoup, T. E., 177
 Skeel, R. D., 496, 513
 Skogestad, S., 443, 458
 Skrifvars, H., 374
 Smith, H., 60, 73
 Smith, J. C., 439, 465, 478
 Smith, S., 306, 320, 328
 Smith, W. K., 565, 581
 Snee, R. D., 254
 Sofer, A., 142, 155, 159, 176, 195, 211, 282, 292, 304, 305, 328
 Sourander, M. L., 254
 Spendley, W., 185, 211
 Srygley, J. M., 443, 458
 Stadtherr, M. A., 543, 546, 548
 Stanley, G. M., 576, 581
 Steihang, T., 195, 210
 Steinberg, D., 177
 Steinmeyer, D. E., 419, 439
 Steur, R. E., 84, 104
 Stevens, W. F., 328, 343
 Stewart, G. W., 584, 598, 600
 Stewart, W. E., 51, 69, 73
 Stichlmair, J., 443, 446, 448, 458
 Stobbe, M., 413
 Stoecker, W. F., 176, 180
 Suh, K., 374
 Sullivan, W. G., 105
 Sung, W., 479
 Swain, J. J., 66, 73
 Swearingen, J. S., 419, 422, 439

 Tarquin, A. J., 105
 Tarrer, A. R., 428, 429, 439
 Ternet, D. J., 329
 Timmer, G. T., 388, 389, 412
 Timmerhaus, K. D., 27, 427, 439
 Tjoa, I. B., 577, 581
 Tomlin, J. A., 253
 Tong, H., 576, 581
 Trachtenberg, I., 501, 503–505, 508, 513
 Trevino-Lozano, R. A., 548
 Tsai, C. L., 84, 104
 Turkay, M., 374, 548
 Turton, R., 329, 604, 610, 629

 Uchiyama, T., 211, 220
 Ulbig, P., 413

 Van Loan, C. F., 584, 596, 600
 Vanderbei, R. J., 223, 242, 253
 Vanston, L. K., 393, 411
 Vasantharajan, S., 548
 Vasquez, M., 496, 513
 Vassiliadis, V. S., 329
 Viswanathan, J., 459

 Wahnschafft, O., 459
 Wajge, R. M., 459
 Walker, W. H., 140, 142
 Wang, K., 413
 Waren, A. D., 306, 313, 328, 360, 373
 Waton, J., 322, 328
 Watson, C. C., 28
 Watson, D. L., 561, 580
 Watson, J., 360, 373
 Watts, D. G., 62, 73
 Waven, A., 322, 328
 Weixnan, L., 177
 Wen, C. Y., 74
 Westerburg, A. W., 319, 328, 372, 459, 517, 529, 542, 546, 547
 Westerlund, T., 374
 White, D. C., 254, 582
 White, J. A., 105
 Whiting, W. B., 604, 610, 629
 Wilde, D. J., 176, 177, 180
 Williams, T. J., 329, 343
 Williamson, C. Q., 253
 Woinsky, S. G., 617, 629
 Wolbert, D., 545, 548
 Wolsey, L. A., 243, 253, 353, 354, 356, 373
 Wood, R. K., 290, 328
 Wright, M. H., 195, 210, 253, 517, 547
 Wright, S. J., 242, 253, 291, 292, 304, 318, 320–322, 328

 Xia, Q., 374
 Xue, G., 496, 513

 Yanniotis, S., 439
 Yeomans, H., 373
 Yocum, F. H., 516, 547

 Zagermann, S., 419, 439
 Zaher, J. J., 526, 548
 Zamora, J. M., 374, 413, 419, 439
 Zhang, J., 298, 301, 329
 Zwick, H., 514

SUBJECT INDEX

- Able to Promise, 554, 565
Active constraint, 229, 274
ADIFOR, 325
Algorithm. *See particular method*
Alkylation reactor, 492
Ammonia synthesis reactor, 488
Amortization, 623
AMPL, 323
Analytical methods. *See also* Necessary and sufficient conditions; Stationary point; Sufficient conditions
 comparison with numerical, 24, 153, 161
 constrained, 267
 computational problems, 162, 164, 175
 continuous functions, 114–151
 examples, 23, 128, 138
 n dimensions, 127, 419, 461, 464
 general conclusions, 128, 132
 one dimension, 23, 135, 161
Analytical models. *See also* Distributed system; Lumped parameter system; Simplification; Surface fitting
 definition, 43
 formulation, 44, 47
 balance equations, 39
 role of mechanisms, 41
 relationship with black box, 42, 48, 54
Applications of optimization, 9, 10, 85, 87, 89, 171, 415–548. *See also* Optimization techniques
Approximation of functions
 linear, 293
 quadratic, 197
Approximation of Hessian matrix, 208, 303
ASCEND, 519
Assignment problem, 252
Augmented Lagrangian methods, 290. *See also* Penalty function methods
Automatic differentiation, 325

Balance sheet, 618, 619, 622
Barrier function, 242, 291
Basic feasible solution in linear programming, 227
 obtaining first basic solution, 233

Basic variables, 227, 307
Basis matrix, 227, 314
Batch process optimization, 560
Batch scheduling, 559
Benders decomposition (MINLP), 370
BFGS method, 208, 304
Binary variable, 352, 407
Binding constraint, 229, 274
Black-box models
 definition, 48, 51
 response surface methods, 62
Blast furnace model, 40
Blending problem, 70
Boiler, 11, 435
Boundaries. *See also* Constraints; Kuhn-Tucker conditions; Penalty function methods; Region of search
 one dimension, 156
 effect on optimum, 168
 and optima, 119, 121, 223
 and slack variables, 226, 284
Bounds, 118, 225
Bracketing procedures, 156
Branch and bound technique, 354
 example, 355, 474
 global optimization, 385
 LP relaxation, 355
 MINLP, 361, 369
 underestimator, 385

Canonical form, 232
Capital cost estimation, 607
Capital costs, 87, 102, 604–610
Case studies for, 416–419, 514
Cash flow, 92, 102, 618, 620
Centroid, 186
Chemical plant optimization, 537
Chemical reactors, 481, 483, 492
 alkylation, 492
 ammonia, 488
 control, 571
 models, 481
 objective functions, 482
 optimal temperature, 482
 simulation, 488

- Chemical reactors—*Cont.*
 - thermal cracker, 484
 - tubular, 488
- Comparison of methods
 - constrained, 318
 - least squares, 55, 61, 577
 - robustness, 318
- Complementary slackness condition, 276
- Compressor, 464
- Computer programs, sources of, 243, 319, 370, 411. *See also particular method*
- Computer-integrated manufacturing, 550
- Concave functions
 - and optimization, 125
- Cone, 273, 274
- Conjugate direction. *See also Fletcher-Reeves method*
 - definition, 187
 - generation, 208, 209
- Conjugate gradient method, 194, 209. *See also Fletcher-Reeves method*
- CONOPT, 370
- Constrained optimization. *See also Nonlinear programming; particular technique*
 - augmented Lagrangian methods, 290
 - computer codes, 319 (*see also particular technique*)
 - diagnosis of failures, 326
 - dynamic processes, 570
 - evaluation, 318
 - generalized reduced gradient method, 306
 - graphical illustration, 267
 - Lagrange multiplier method, 278
 - necessary and sufficient conditions, 281
 - penalty functions, 285
 - quadratic programming, 284
 - successive quadratic programming, 302
 - successive linear programming, 293
- Constrained optimum, 265
- Constraint qualification, 271
- Constraints. *See also Global optimization*
 - active, 229, 274
 - binding, 229, 274
 - definition, 15, 16
 - degrees of freedom, 15, 229, 294, 427, 520–523
 - equality, 271, 273
 - inequality, 15, 226
 - linear, 223
 - nonlinear, 265
 - physical basis, 39, 41, 68, 70, 71
 - removal, 265
- Continuous variables, 114, 116
- Contours, definition of, 132, 136
- Control, 568
- Control moves, 570
- Convergence rate. *See also specific methods*
 - linear, 157
 - Newton's method, 158
 - order, 157
 - quadratic, 157
 - superlinear, 158
- Convex functions
 - definition, 122
 - Hessian matrix, 128
 - linear case, 128
 - optimization, 266, 280
- Convex programming problem, 280
- Convex region (sets), 124
- Cost estimation, 606–614
- Cost index, 612–614
- Costs
 - investment capital, 93, 99, 102, 604–614
 - operating, 85, 89, 102, 610–611
- Criterion of selection, 5. *See also Objective function; Profit*
- Crude oil, 556
- Cross-current extraction, 448
- Cubic interpolation, 169
- Curve fitting, 42, 51, 56, 62
- Cyclical, 540
- Cycling, 239
- Data reconciliation, 576
- Debt-equity ratio, 626
- Decision variable. *See Variable(s), independent*
- Decomposition. *See also Hessian matrix*
 - complex system, 540
 - generalized Benders, 370
 - MINLP, 361
 - need for, 19
- Degeneracy in linear programming, 239
- Degenerate vertex, 229
- Degrees of freedom, 66, 229, 294, 427, 520–523
- Dependent variable, 232, 308
- Depletion, 622
- Depreciation, 623–624
 - comparison of methods, 624
 - definition, 623
 - MACRS, 623
 - straight-line, 623
- Derivative-free methods, 183, 325. *See also Finite difference substitutes for derivatives*
- Derivatives
 - approximation, 324 (*see also Finite difference substitutes for derivatives*)
 - optimization, discontinuities, 115
 - in simulators, 544

- Design, 516, 517
- Design costs, 606
- Design of experiments. *See* Experimental design
- Determinants, 589
 - definition, 589
- Deviation variable, 289
- Diagnosis of causes of failure of optimization codes, 326
- DICOPT, 369
- Direct methods
 - comparison of one-dimensional, 161, 163
 - conjugate search directions, 186
 - discrete-valued functions, 428
 - Nelder-Mead, 186
 - one dimension, 152–180
 - acceleration, 156
 - fixed step size, 156
 - polynomial approximation, 166
 - random search, 183
 - simplex search, 185
- Direct substitution
 - equality restrictions, 225, 265
 - slack variables, 226
- Direction of search. *See also* Conjugate direction; Steepest ascent; *specific methods*
 - conjugate, 187
 - parametric representation, 174
- Discontinuities, 114
 - effect of function, 114, 124
- Discounted cash flow, 91, 94, 100
- Discrete event dynamic systems, 565
- Discrete-valued objectives, 115, 116. *See also* Integer programming
- Disjunctive programming, 371
- Distillation (staged)
 - decision parameters, 443
 - examples, 443, 451, 453
 - extraction, 546
 - optimal design, 443
 - optimal reflux, 11, 453
- Distributed system
 - definition, 44
 - difference from lumped parameter, 45
- Eigenvalue of Hessian matrix, 128, 132, 598
- Eigenvector associated with Hessian matrix, 135, 598
- Electrostatic precipitator model, 41
- Energy conservation, 89, 102, 418
- Enterprise Resource Planning (ERP), 553
- Equality constraints. *See also* Slack variables
 - origin, 14, 38
 - SQP formulation, 302
- Equation-based optimization, 518–519, 524–525, 536
- Equations. *See* Constraints
- Equipment costs, 606
- Equipment replacement policies. *See* Depreciation
- Equity, 626
- Error in measurement, 577
- Error in numerically evaluated derivatives, 324
- Evaluation of algorithms. *See* Comparison of methods
- Evaporator, 430
- Evolutionary solver, 400
- Excel Solver
 - in LP, 245
 - in MILP, 363
 - in NLP, 322
- Expense statement, 618, 620
- Expenses, 621
- Experimental design. *See also* Factorial experimental designs
 - number of experiments, 63
 - orthogonal design, 62
- Extraction example, 448
- Extractive distillation, 546
- Extrema. *See* Optima
- Factorial experimental designs
 - two-level, orthogonal, 63
- Fathom (in branch and bound), 356
- Feasibility, 119–124, 239
- Feasible direction, 274
- Feasible points, 119–124, 239
- Feasible region, 119, 223
- Filter, 466
- Financial statements, 618
- Finite difference substitutes for
 - derivatives, 324
 - in flowsheeting simulations, 544–545
- Fitness (in genetic algorithms), 401
- Fitting models to data, 48
- Fletcher-Reeves method
 - algorithm, 194
 - example, 196
- Flowsheet codes, 518–520
- Flowsheet optimization, 518–546
- Fluid flow examples, 461
- Full vector, 524
- Function(s)
 - approximation of (*see* Approximation of functions)
 - concave, 123, 125
 - continuous, 114
 - convex, 122, 125

- Function(s)—*Cont.*
 discontinuous, 114
 discrete, 115, 352 (*see also* Concave functions; Convex functions; Unimodal functions)
 objective, 84
 quadratic, 55, 84, 284 (*see also* Quadratic function)
 unbounded, 225
 unimodal, 155
 Future worth, 94
- GAMS, 323
 Gas compression, 464
 Gas pipeline, 469
 General polynomials
 form, 55
 n -dimensional, first degree, 55
 quadratic, 56, 587
 Generalized Benders decomposition (GBD), 370. *See also* Surface fitting, quadratic surfaces, for optimization
 Generalized reduced gradient (GRG), 306
 algorithm, 306, 527
 codes, 320
 reduced gradient, 308
 refrigeration process, 530
 Genetic algorithms, 400
 Global optimization, 382
 branch and bound, 385
 evolutionary, 400
 metaheuristics, 382
 multistart methods, 388
 scatter search, 408
 simulated annealing, 399
 tabu search, 393
 Global optimum, 121, 127, 132
 Gradient method, 189
 convergence, 192
 definition, 189
 evaluation, 207
 oscillation, 192
 reduced, 308
 steepest descent, 190
 step length, 191
 Gradient search, 189. *See also* Conjugate direction; Fletcher-Reeves method; Gradient method
 GRG, 306. *See also* Generalized reduced gradient
 GRG2, 320
 Grid search, 183
 Gross error detection, 576
 Heat exchange, 252, 418, 419–450
 Heat exchanger, 419, 422
 cost estimation, 609
 networks, 252
 Heat transfer, 418
 Hessian matrix
 approximation of, 208
 Cholesky factorization, 203
 eigenvalues of, 128, 132, 598
 eigenvectors for, 135, 598
 inverse, 202
 positive definite, 598
 Hierarchy of optimization, 6
 Hill climbing. *See* Gradient method
 Horizon, 571
- Income statement, 618, 620, 622
 Income taxes, 625
 Independent variables, 15
 Indexes, 612–614
 Inequality constraints
 form, 223
 transformation to equality constraints, 226
 Inflation, 611–614, 625
 Initial solution, 240
 Insulation thickness, 10, 89, 102
 Integer programming
 branch and bound technique, 354
 computer codes, 243, 352
 Interaction among variables, 192
 Interest rate, 94, 97, 100
 Interior point, 242–291
 Internal rate of return, 100, 102
 Inverse Hessian matrix. *See* Hessian matrix
 Investment. *See* Costs
 IRR, 615, 617. *See also* Internal rate of return
 Irreducible nets, 540
- Jacobian, 294, 598
 Job scheduling, 560
- Kalman filter, 577
 Karush-Kuhn-Tucker conditions, 267
 Knapsack problem, 352
 Kuhn-Tucker conditions, 267
- Lagrange multipliers, 271
 interpretation, 273
 Lagrangian function, 271
 Large-scale optimization, 323
 Least squares. *See also* Experimental design
 applications, 58, 61, 63, 577
 definition, 55, 61, 577
 examples, 58, 59, 451

- n dimensions, linear surface, 55
 - necessary conditions, 57
 - optimization technique, 57
 - orthogonal design, 62
- Levels of optimization, 6
- Levenberg Marquardt method, 202. *See also specific method*
- Line search, 155, 173, 193. *See also Unidimensional search*
- Linear dependence, 593
- Linear equations, 595
- Linear independence, 593
- Linear model, 55, 223
- Linear objective function, 223
- Linear programming, 223
 - applications, 252
 - assignment problems, 252
 - basic solution, initial, 227
 - basis matrix, 227
 - canonical system, 232
 - computer codes, 243
 - degeneracy, 239
 - examples of, 245, 435
 - mixed integer programs, 243
 - modeling systems, 243
 - network flow, 252
 - phase I-phase II, 239
 - pivoting, 230
 - sensitivity analysis, 242
 - simplex method, 233
 - software, 243
 - standard LP form, 225
 - successive (in NLP), 293
 - transportation problems, 245
 - unboundedness, 238
- Linear regression. *See* Least squares
- Linearization
 - definition of linear system, 43
 - techniques, 293
- Liquid-liquid extraction. *See* Extraction example
- Lithography example, 171
- Local optima, 327, 382
- Location problem, 354
- Logarithmic barrier function, 291
- LSGRG2, 320
- Lumped parameter system
 - definition, 44
 - difference from distributed, 44
- MACRS, 623
- Manufacturing problem, 20
- Manipulated variable, 569
- Marquardt's method, 202
 - example, 203
- Material balance reconciliation, 17, 578
- Mathematical models, 37–82
- Mathematical programming, 223
- Matrix
 - basis, 227
 - condition number, 598
 - definitions, 584
 - determinant, 598
 - eigenvalues, 598
 - Hessian, 592 (*see also* Hessian matrix)
 - identity, 584
 - indefinite, 127
 - inverse, 596
 - Jacobian, 592
 - negative definite, 127
 - notation, 584
 - occurrence, 530
 - operations, 585
 - positive definite, 127, 598
 - principal minors, 589
 - rank, 594
 - semidefinite, 127
 - symmetric, 132, 584
 - transpose, 587
 - variance-covariance, 577
- Maxima. *See* Optima; Sufficient conditions
- Measurement error, 577
- Metaheuristics, 382
- Metropolis algorithm, 399
- MILP, 243, 354
- Minima. *See also* Constrained optimum; Necessary and sufficient conditions; Optima; Sufficient conditions
 - global, 118, 121, 138
 - local, 118, 123, 138
- Minimization
 - in a search direction, 133
 - unconstrained (*see* Unconstrained optimization)
- MINOS, 321
- Mixed integer linear programming, 243, 352
- Mixed integer nonlinear programming, 361
- Mixed integer programming. *See also* Integer programming
 - computer codes, 243
 - nonlinear, 361
- Model Predictive Control, 568
- Modeling systems, 322, 323
- Models. *See also* Analytical models; Black-box models; Process simulators
 - chemical reactions, 481
 - classification, 43
 - forms, 43, 48, 49
 - manufacturing, 21, 552
 - model-building, 46, 49
 - plant optimization hierarchy, 551, 553

- Modified objective function
 - Lagrangian formulation, 271
 - penalty function, 285
- Modular-based optimization, 519, 534, 537
- Module, 518, 537
- Monitoring, 575
- MPL, 323
- Multimodal functions, 135, 138
- Multistage processes, 561
- Multistart method, 388
- Mutation (in genetic algorithm), 401
- Necessary and sufficient conditions
 - first order, 128, 137
 - functions of continuous variables
 - constrained, 267
 - example applications, 269 (*see also* Kuhn-Tucker conditions; Lagrange multipliers)
 - second order, 281
 - unconstrained, 137
- Need for optimization, 4
- Negative definite, 128
- Nelder-Mead method, 186
- Nesting, 541
- Net present value, 100, 102, 615, 617
- Networks
 - generalized, 353
 - heat exchanger, 252
 - pipeline, 158, 469
- Newton-Raphson method, 197, 597
- Newton's method, 197. *See also* Quasi-Newton methods
 - advantages, 158, 161, 202
 - algorithm, 158
 - convergence, 161
 - direction of search, 197
 - disadvantages, 202
 - example, 199
 - geometric interpretation, 198
 - modified, 202
 - of solving equations, 597
 - step length, 197
- NLP (nonlinear programming) algorithm
 - advantages of different methods, 318
- NLPQL, 321
- Nodes (branch and bound), 355
- Nonlinear constraints, 265
- Nonlinear equations, solution of, 598
- Nonlinear model, 49
- Nonlinear programming problem. *See also* Constrained optimization; Unconstrained optimization
 - convex, 280
 - definition of, 265
 - example of, 267
 - geometric illustration, 268
- Nonlinear regression, 61, 451
- NPSOL, 321
- NPV. *See* Net present value
- Numerical evaluation of derivatives. *See* Finite difference substitutes for derivatives
- Numerical search
 - comparison, 161
 - n dimensions
 - examples, 465
 - one dimension, 152–180
 - direct methods, 166
 - examples, 161, 163, 168, 171, 431, 443, 466
 - indirect methods, 161
 - stopping criteria, 161, 168, 234, 326
- Objective. *See also* Linearization; Simulation
 - definition, 19, 84
 - economic criteria, 7, 19, 100
 - investment costs, 89, 93, 100, 604–610
 - operating costs, 85, 100, 610–611
 - profit, 100, 621, 622
- Objective function. *See also* Linearization
 - chemical reactors, 482
 - contours, 132
 - form, 131
 - linear, 223
 - simplification, 19
- Off-line optimization, 524
- Oil well location, 354
- Olefin production, 484
- One-dimensional search. *See* Numerical search; Unidimensional search
- On-line optimization, 524
- Operating cost estimation, 610
- Operating expenses, 621, 622
- Optima
 - boundaries, 119, 124 (*see also* Necessary and sufficient conditions; Stationary point)
 - conditions, 118, 126
 - existence, 118, 126
 - global, 121, 127, 132
 - local, 121, 127, 132
 - multiple extrema, 135, 382
 - n dimensions, 118
 - restricted, 121–124 (*see also* Direct substitution; Lagrange multipliers; Linear programming; Penalty function; Slack variables)
 - unrestricted, 125, 132
- Optimal control, 568
- Optimal point, 118
- Optimal scheduling, 560, 565

- Optimal solution, 14
- Optimal value. *See* Optimal solution
- Optimization
 - difficulties, 26, 326
 - essential features, 14
 - general procedure, 19
 - need for, 4
 - objectives of, 4
 - obstacles to, 26
 - off-line, 524
 - on-line, 524
 - six steps, 19, 20
 - strategies, 19, 265
- Optimization characteristics. *See also* Levels of optimization
 - comparison of numerical and analytical, 23
 - general procedure, 18
 - iteration, 182
 - need for optimization, 4
 - objectives, 4
 - opposing influences, 10, 11, 12
- Optimization complexity. *See also* Levels of optimization
 - dimensionality, 19
- Optimization software, 518–520, 525
- OPTQUEST, 409
- Ordinary differential equations, 49
- Orthogonal search directions, 188
- Oscillation, 192, 299
- Outer approximation (MINLP), 369

- Parametric penalty function methods, 290
- Parametric representation, 52, 55
- Parameter estimate, 55, 58
- Payback period, 100
- Payout time, 100
- Penalty function, 285
 - size of penalty, 288
- Penalty function methods
 - algorithm, 285
 - ill-conditioning, 286 (*see also* Lagrange multipliers)
- Penalty parameter, 285
- Penalty SLP algorithm, 298
- Phase I-Phase II procedure, 239
- Pipe diameter, 461, 469
- Planning, 553
- Plant optimization, 537
- Plant optimization hierarchy, 6, 550
- Plantwide management and optimization, 565
- Point
 - feasible, 15, 118
 - saddle, 127, 132, 135
 - stationary, 127, 132, 135, 267

- Polynomials. *See* General polynomials; Surface fitting
- Positive definite, 128, 132, 598
- Positive-definite Hessian matrix, 128, 132, 304
- Positive-definite matrix, 128, 598
- Positive-semidefinite matrix, 128, 132
- Precedence ordering, 539
- Prediction horizon, 570
- Present value (worth), 94, 100
- Pressure vessel optimization, 87
- Problem formulation, 19
- Process design, 6, 516–517
- Process monitoring and analysis, 575
- Process operations, 551
- Process selection, 400
- Process simulators, 518–520
- Profit, 621, 622
 - chemical plant, 85
 - investment/profit criteria, 100
- Profitability measures, 100, 615
- Programs, computer, 243, 370
- Project evaluation, 615
- Project life, 616, 623

- Quadratic approximation, 197, 302
 - geometric interpretation, 198
- Quadratic convergence, 157, 200. *See also* Conjugate direction
- Quadratic form, 132, 197
- Quadratic function
 - coefficient estimation, 55, 60 (*see also* Surface fitting)
 - conjugacy, 187
 - geometry, 132
 - minimization, 132, 187
- Quadratic interpolation, 166
- Quadratic programming, 284
 - codes, 285
 - quadratic programming problem, 284, 571
- Quasi-Newton methods
 - algorithm, 160, 208
 - BFGS, 208
 - examples, 161, 163, 209
 - movement in search direction, 208
 - unidimensional, 160
 - updating Hessian matrix, 208

- Random search methods, 183
- Rate of return. *See* Internal rate of return
- Reaction synthesis, 508
- Reactive scheduling, 553
- Reactors, chemical. *See* Chemical reactors
- Real-time optimization (RTO), 524, 565
- Recursive quadratic programming. *See* Successive quadratic programming

- Recycle systems, 509
- Reduced gradient, 308
- Reduced gradient method, generalized, 306
- Reduced vector, 524
- Reduction, 19
- Refinery application, 556
- Reflection, 187
- Reflux ratio, 443
- Refrigeration process, 530
- Region. *See* Feasible region
- Region of search, 118, 124, 274. *See also*
 - Boundaries; Constraints
 - interior optima, 118, 291
 - nonconvex, 327
- Regression. *See* Least squares
- Relative sensitivity, 25
- Repayment multiplier, 95
- Residual, 57
- Return on investment, 100
- Revenues, 614, 621
- ROI, 100
- Rosenbrock's function, 196
- Roundoff error, 324

- Saddle point
 - one dimension, 135
 - two dimensions, 127, 132
- Safeguarded Newton's method, 207
- Sales, 7
- Salvage value, 625
- Scaling, 327
 - flowsheet optimization, 526, 532
 - in one-dimensional search, 155
- Scanning (unidimensional search), 156
- Scatter search, 408
- Scheduling problem, 560
- Search methods. *See specific method*
- Secant methods. *See* Quasi-Newton methods
- Second derivatives, 127, 132, 197, 303
- Second-order-necessary conditions, 281
- Sensitivity, 25, 242, 279
- Separations processes, 441–459. *See also*
 - Distillation (staged); Extraction example
- Sequential modular flowsheeting, 524, 539
- Sequential quadratic programming. *See* Successive quadratic programming
- Sequential search
 - discrete-valued objectives, 115, 116
 - one-dimensional search, 156, 168
 - simplex, 185
- Shadow price, 242, 279. *See also* Lagrange multiplier
- Simplex, 185, 233
- Simplex method of search, 185. *See also* Linear programming
- Simplification. *See also* Decomposition; Linearization; Objective function
 - linear approximation, 19, 293
 - mathematical, 19
 - physical model, 21, 47
 - quadratic approximation, 131, 302
- Simulated annealing, 399
- Simulation, 518–520
 - sequential modular, 524, 529
 - simultaneous modular, 524, 527, 543
- Simultaneous modular model, 524, 527, 543
- Slack variables, 225
 - inequality constraints, 223
- Lagrange multipliers, 269 (*see also* Kuhn-Tucker conditions)
- linear systems, 230
- sufficient conditions, 281
- Software
 - flowsheeting simulators, 544–545
 - global optimization, 411
 - LP, 223
 - MILP, 243
 - MINLP, 370
 - NLP, 319
- Spreadsheet optimizer, 243, 322
- Spreadsheets, 243, 322
- SQP. *See* Successive quadratic programming
- Stationary point, 269
 - definition, 282
 - n dimensions, 259
 - constrained, 282
 - Kuhn-Tucker conditions, 269
 - unconstrained, 127
 - one dimension, 135
 - need for higher derivatives, 135
- Steady state model, 44
- Steam generator, 435
- Steam system, 435
- Steepest ascent. *See* Gradient method
- Steepest descent. *See* Gradient method
- Step response, 570
- Step response model, 570
- Step size in search, 156, 158, 160, 190, 304, 311. *See also specific method*
- Stopping criteria. *See* Termination
- Strictly concave, 123
- Strictly convex, 123
- Suboptimization, 8
- Successive linear programming, 293
- Successive quadratic programming
 - algorithm, 302

- codes, 321
- examples, 305
- Sufficient conditions, 281. *See* Necessary and sufficient conditions
- Sum of infeasibilities, 240, 315
- Superbasic variables, 310
- Superposition, 43
- Supply chain management, 550
- Supply limit, 556
- Surface fitting, 54, 62
 - definition, 55
 - "fit", 56. *See* Least squares
 - quadratic surfaces, 55
 - for optimization, 59
- Synthesis, 516
- Tabu search, 393
- Tax credit, 625
- Taxes, 625
- Taylor series, 136
- Tearing, 540, 541
- Termination, 194, 305, 325. *See also*
 - Convergence rate
- Thermal cracker, 484
- Time value of money, 94
- Transformation method. *See* Penalty function
- Transportation problem, 245
- Traveling salesman problem, 353
- Trust region, 206, 298
- Two-level experiment design, 184. *See* Factorial experimental designs
- Unconstrained optimization, 183
 - examples, 204, 209, 451, 464
- Underestimator, 385
- Unidimensional search
 - indirect, 155, 157
 - interpolation, 166
 - multidimensional search, 173
 - polynomial approximation, 166
 - scanning and bracketing procedures, 156
- Unimodal functions
 - definition, 156
 - in numerical search, 156
- Unit management and control, 567
- Univariate search, 185
- Unsteady state model, 44, 569
- Upper bounded variables, 225, 299
- Vapor-liquid equilibrium, 451
- Variable(s)
 - basic, 227
 - continuous *versus* discrete, 352
 - dependent, 232, 308
 - independent, 232, 308
 - interaction among, 131
 - nonbasic, 232, 308
 - slack, 226, 284
- Variance-covariance matrix, 577
- Vector, 524, 584
- Vertex, linear equalities, 229
- Waste heat recovery, 419
- Weighting factor, 571
- Yield matrix, 484

