Algorithms for Constrained Optimization: The Benefits of General-purpose Software

Michael Saunders
MS&E and ICME, Stanford University, California, USA

ICME LA/Opt seminar, January 24, 2024

Abstract

Algorithms for Constrained Optimization: The Benefits of General-purpose Software

We review the history of numerical optimization at the Systems Optimization Laboratory (SOL) instituted in 1974 by Professors George Dantzig and Richard Cottle within Stanford's Dept of Operations Research.

We describe some unexpected applications of optimization software within aerospace, radiotherapy, signal analysis, systems biology, and economics.

Sometimes general-purpose software leads to new applications. Sometimes new applications lead to new algorithms (which we implement with general-purpose software).

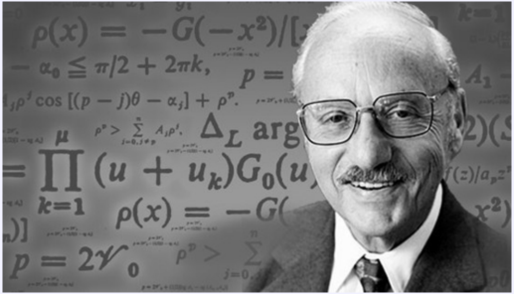
SOL

Systems Optimization Laboratory
Stanford University

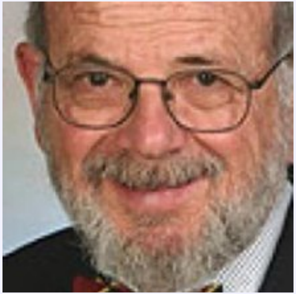
On the Need for a System Optimization Laboratory
George B. Dantzig, R.W. Cottle,
B.C. Eaves, F.S. Hillier, A.S. Manne,
G.H. Golub, D.J. Wilde, and R.B. Wilson

Mathematical Programming **(book, 1973)**
T.C. Hu and Stephen M. Robinson (editors)

SOL Founded 1974 by George Dantzig and Richard Cottle



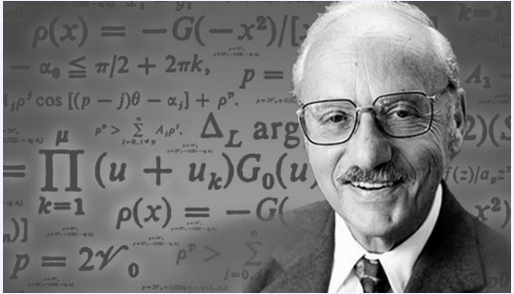
George Dantzig
1914–2005



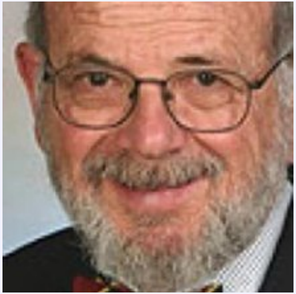
Richard Cottle
1934–

Alan Manne
1925–2005

SOL Founded 1974 by George Dantzig and Richard Cottle



George Dantzig
1914–2005

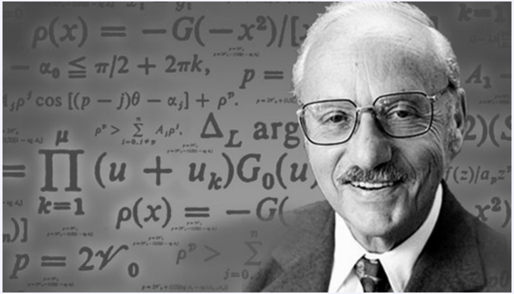


Richard Cottle
1934–

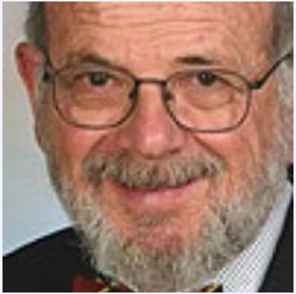
Alan Manne
1925–2005

1974–2005 Dantzig PILOT Economic models linear programs

SOL Founded 1974 by George Dantzig and Richard Cottle



George Dantzig
1914–2005

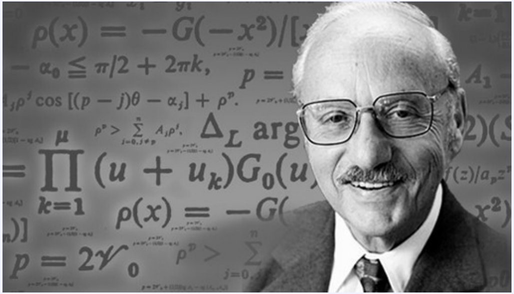


Richard Cottle
1934–

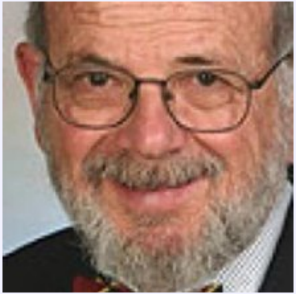
Alan Manne
1925–2005

1974–2005 Dantzig	PILOT Economic models	linear programs
	PILOTJA	Several $0 \le x_j \le 10^{-5}$!!

SOL Founded 1974 by George Dantzig and Richard Cottle



George Dantzig
1914–2005

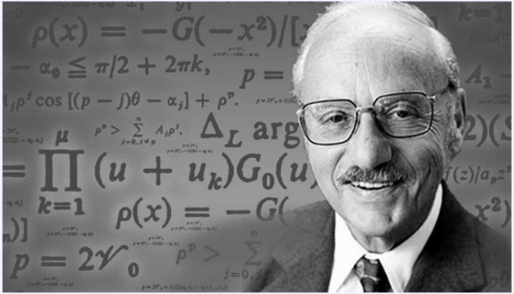


Richard Cottle
1934–

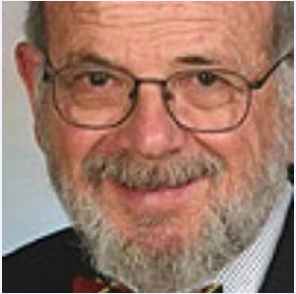
Alan Manne
1925–2005

1974–2005 Dantzig	PILOT Economic models	linear programs
	PILOTJA	Several $0 \le x_j \le 10^{-5}$!!
1974–2005 Alan Manne	ETAMACRO	nonlinear objective

SOL Founded 1974 by George Dantzig and Richard Cottle



George Dantzig
1914–2005



Richard Cottle
1934–

Alan Manne
1925–2005

1974–2005 Dantzig	PILOT Economic models PILOTJA	linear programs Several $0 \le x_j \le 10^{-5}$!!
1974–2005 Alan Manne	ETAMACRO COBB-DOUGLAS Test problems for MINOS	nonlinear objective nonlinear constraints

General-purpose software for optimization

Linear programming

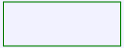
Textbook: $$\min_x \; c^T x \quad \text{st} \quad Ax = b,\; x \geq 0 \qquad A = \boxed{}$$

Linear programming

Textbook: $\min_x \; c^T x \quad \text{st} \quad Ax = b, \; x \geq 0 \qquad A = \boxed{}$

Useful software: $\min_x \; c^T x \quad \text{st} \quad \ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u \qquad A$ any shape

Linear programming

Textbook: $\min_{x} \; c^T x \quad \text{st} \quad Ax = b, \; x \ge 0$ $\qquad A =$ 

Useful software: $\min_{x} \; c^T x \quad \text{st} \quad \ell \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$ $\qquad A$ any shape

Implementation: $\min_{x,s} \; c^T x \quad \text{st} \quad Ax - s = 0, \quad \ell \le \begin{pmatrix} x \\ s \end{pmatrix} \le u$

Linear programming

Textbook: $\min_{x} c^T x \quad \text{st} \quad Ax = b,\ x \geq 0 \qquad A = \boxed{}$

Useful software: $\min_{x} c^T x \quad \text{st} \quad \ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u \qquad A \text{ any shape}$

Implementation: $\min_{x,s} c^T x \quad \text{st} \quad Ax - s = 0, \quad \ell \leq \begin{pmatrix} x \\ s \end{pmatrix} \leq u$

A is sparse because it might be big!

Some history: 1970s, 1980s, 1990s, . . .

1975 Dantzig and President Ford: National Medal of Science

Gang of 4, 1979–1988

Optimization problems

Minimize an objective function subject to constraints:

$$\min\ \varphi(x) \quad \textbf{st} \quad \ell \le \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \le u$$

x	**variables**	
A	**matrix**	
$c(x)$	**nonlinear functions**	$\begin{pmatrix} c_1(x) \\ \vdots \\ c_m(x) \end{pmatrix}$
ℓ, u	**bounds**	

Ideally we know the gradients of $\varphi(x)$ and the Jacobian of $c(x)$

1970s

SOL history

1974	Dantzig and Cottle start SOL
1974–78	John Tomlin: LP/MIP expert
1974–2005	Alan Manne: nonlinear economic models
1975–76	MS and Bruce Murtagh: MINOS first version (LP + nonlinear objective)

SOL history

1974	Dantzig and Cottle start SOL
1974–78	John Tomlin: LP/MIP expert
1974–2005	Alan Manne: nonlinear economic models
1975–76	MS and Bruce Murtagh: MINOS first version (LP + nonlinear objective)
1979–87	Philip Gill, Walter Murray, MS, Margaret Wright (Gang of 4!)
1978–81	Gill, Murray, Wright: *Practical Optimization*
1980–	G4: QPSOL, LSSOL, NPSOL
1982–	MS and Bruce Murtagh: MINOS second version (nonlinear constraints)

SOL history

1974	Dantzig and Cottle start SOL
1974–78	John Tomlin: LP/MIP expert
1974–2005	Alan Manne: nonlinear economic models
1975–76	MS and Bruce Murtagh: MINOS first version (LP + nonlinear objective)
1979–87	Philip Gill, Walter Murray, MS, Margaret Wright (Gang of 4!)
1978–81	Gill, Murray, Wright: *Practical Optimization*
1980–	G4: QPSOL, LSSOL, NPSOL
1982–	MS and Bruce Murtagh: MINOS second version (nonlinear constraints)
1989–	Gerd Infanger: stochastic optimization
2002–	Yinyu Ye: optimization algorithms, especially interior methods

SOL history

1974	Dantzig and Cottle start SOL
1974–78	John Tomlin: LP/MIP expert
1974–2005	Alan Manne: nonlinear economic models
1975–76	MS and Bruce Murtagh: MINOS first version (LP + nonlinear objective)
1979–87	Philip Gill, Walter Murray, MS, Margaret Wright (Gang of 4!)
1978–81	Gill, Murray, Wright: *Practical Optimization*
1980–	G4: QPSOL, LSSOL, NPSOL
1982–	MS and Bruce Murtagh: MINOS second version (nonlinear constraints)
1989–	Gerd Infanger: stochastic optimization
2002–	Yinyu Ye: optimization algorithms, especially interior methods
1996–	G3: SNOPT, QPOPT, NPOPT (now G2: Philip Gill, Elizabeth Wong, UCSD)
2014–	MS, Ding Ma: QuadMINOS, DQQ procedure
2017–	MS, Ding Ma, Ken Judd, Dominique Orban: Algorithm NCL
2019	UC Berkeley opened George B. Dantzig Auditorium

1970s

- MS and Bruce Murtagh: MINOS solver (nonlinear objective)
- George Dantzig: PILOT economic model of US (LP)
- Alan Manne: ETAMACRO energy model (nonlinear objective)

1980s

1980s

- MINOS solver (sparse nonlinear constraints)
- NPSOL solver (dense nonlinear constraints), SQP method

- Optimal Power Flow @ General Electric
- Aerospace optimization @ NASA Ames, McDonnell-Douglas

1990s

1990s

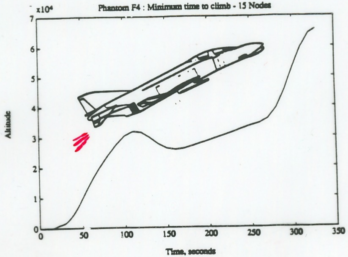
- Alan Manne: MERGE greenhouse-gas model (sparse nonlinear constraints)

1990s

- Alan Manne: MERGE greenhouse-gas model (sparse nonlinear constraints)
- Philip Gill: Aerospace trajectory optimization @ McDonnell-Douglas, LA
  F-4 Minimum time-to-climb
  DC-Y SSTO Minimum-fuel landing maneuver

Aerospace Applications
of NPSOL and SNOPT

OTIS #1



Start at sea-level

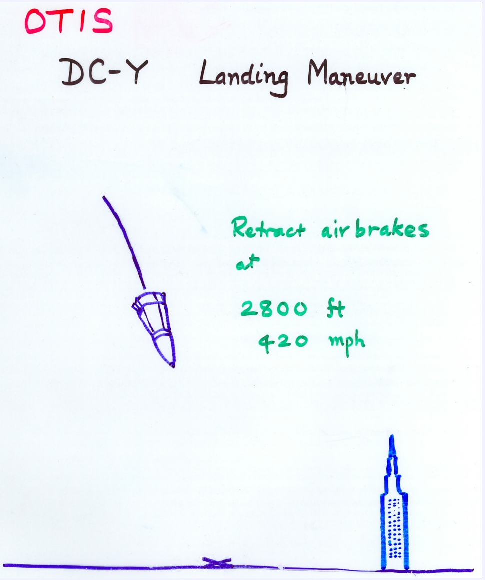
Climb to 65,000ft
Speed Mach 1

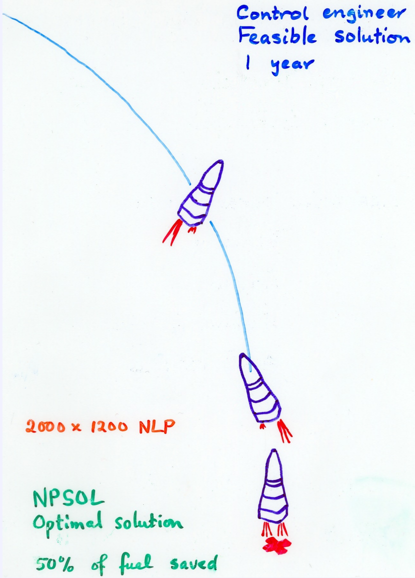
DC-X prototype 1990s: Successful take-off and landing

1/3 full-size = 40ft tall

DC-Y single-stage-to-orbit full-size

← Taking-off?
Landing?


OTIS
DC-Y Landing Maneuver
Retract airbrakes
at
2800 ft
420 mph


Control engineer
Feasible solution
1 year
2000 x 1200 NLP
NPSOL
Optimal solution
50% of fuel saved

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed:

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

Optimum starting altitude = 450m(!)

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

Optimum starting altitude = 450m(!)

Come back Alan Shepard!

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

Optimum starting altitude = 450m(!)

Come back Alan Shepard!

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

Optimum starting altitude = 450m(!)

Come back Alan Shepard!

1961 Mercury-Redstone 3 (suborbital)
First American astronaut 21 days after Yuri Gagarin orbited the Earth

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft ≈ 900m
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

Optimum starting altitude = 450m(!)

Come back Alan Shepard!

1961 Mercury-Redstone 3 (suborbital)
First American astronaut 21 days after Yuri Gagarin orbited the Earth

1971 Commander of Apollo 14 (33 hours on the moon)
First person to play golf on the moon

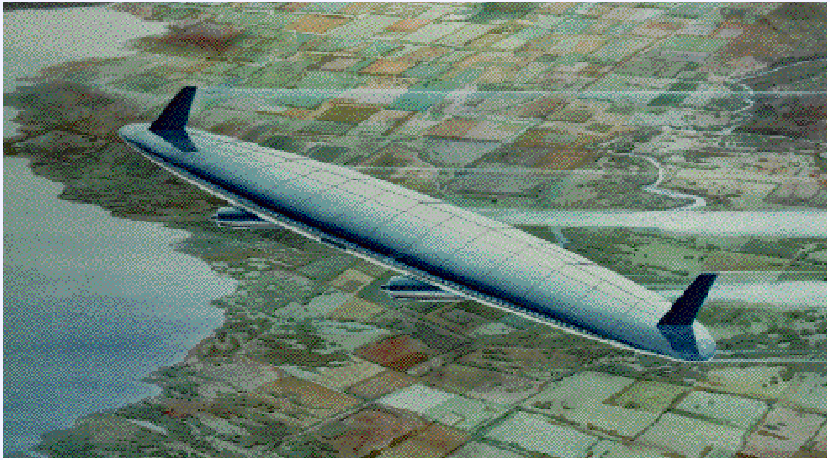
2000s

2000s

David Saunders, NASA Ames (Calif)

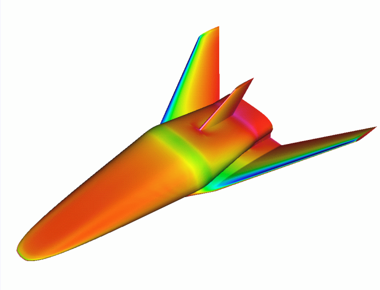
- Wǒ shuāng bāotāi!
  1970: visit Stanford for 6 weeks
  2023: 50 years at NASA Ames
- Shape optimization
  Supersonic airliners
  Heat shield for Mars Landers, Orion
- Trajectory optimization
  SHARP (next Space Shuttle)

OAW oblique all-wing airliner



HSCT high speed civil transport

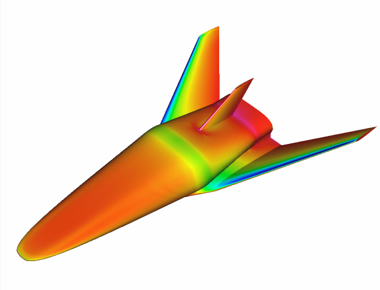
CTV crew transfer vehicle



SHARP design (Slender Hypervelocity Aerothermodynamic Research Probes)

Aerothermal performance constraint in (Velocity, Altitude) space, used during trajectory optimization with UHTC materials (Ultra High Temperature Ceramics) to avoid exceeding material limits

CTV crew transfer vehicle



SHARP design (Slender Hypervelocity Aerothermodynamic Research Probes)

Aerothermal performance constraint in (Velocity, Altitude) space, used during trajectory optimization with UHTC materials (Ultra High Temperature Ceramics) to avoid exceeding material limits

- Trajectory optimization with SNOPT
- Could always abort to Kennedy Space Center, Boston, Gander (Newfoundland), or Shannon (Ireland)

Image credit: David Kinney, NASA Ames Research Center

2010s

2010s

David Saunders, NASA Ames (Calif)

- Orion
  Apollo-type capsule to ISS and moon
- MSL (Mars Science Lab)
  Heat flux during atmospheric entry
- Stratolaunch
  Descent trajectory of space vehicle

Crew Exploration Vehicle (Orion)

- Shape optimization of heat shield and shoulder curvature
- The Apollo designers got it right!

Stratolaunch carrier aircraft (first flight April 15, 2019)

AIAA 2018

018-5257

Fig. 2 Stratolaunch carrier aircraft.

Stratolaunch carrier aircraft (first flight April 15, 2019)

Landing of launched space vehicle

- Preliminary computation: Space vehicle will land in Mojave Desert, California
- OTIS trajectory optimization: Vehicle would land 2500km too soon!

AIAA 2018

018-5257

Fig. 2 Stratolaunch carrier aircraft.

Signal analysis using PDCO

Primal-Dual interior method for Convex Objective

General-purpose MATLAB software

$$\min_{x,r} \ \varphi(x) \ \text{ st } \ Ax + Dr = b, \ \ \ell \le x \le u$$

Signal analysis using PDCO

Primal-Dual interior method for Convex Objective

General-purpose MATLAB software

$$\min_{x,r}\ \varphi(x) \ \text{ st }\ Ax + Dr = b,\ \ \ell \le x \le u$$

Unique feature: A may be a linear operator $(Av, A^T u)$

Search directions computed by iterative method LSQR or LSMR

Signal analysis using PDCO

Primal-Dual interior method for Convex Objective
General-purpose MATLAB software

$$\min_{x,r} \ \varphi(x) \ \text{ st } \ Ax + Dr = b, \ \ \ell \le x \le u$$

Unique feature: A may be a linear operator $(Av, A^T u)$
Search directions computed by iterative method LSQR or LSMR

- 1998 BPDN: Basis Pursuit DeNoising — Shaobing Chen, David Donoho, MS (Stanford)
  $\varphi(x) = \|x\|_1$, A is a dictionary of FFTs, wavelets, ...

Signal analysis using PDCO

Primal-Dual interior method for Convex Objective

General-purpose MATLAB software

$$\min_{x,r} \; \varphi(x) \; \text{ st } \; Ax + Dr = b, \;\; \ell \le x \le u$$

Unique feature: A may be a linear operator $(Av, A^T u)$

Search directions computed by iterative method LSQR or LSMR

- 1998 BPDN: Basis Pursuit DeNoising — Shaobing Chen, David Donoho, MS (Stanford)
  $\varphi(x) = \|x\|_1$, A is a dictionary of FFTs, wavelets, ...
- 2011 1D LF-NMR (Low-Field NMR analysis) — Ofer Levi, MS, S. Berman, Z. Wiesman (Israel)
- 2018 2D LF-NMR

2D LF-NMR analysis using PDCO

Analysis of biodiesel, olive oil, . . .

$$\begin{array}{ll} \min_{f,r} & \lambda_1 \|f\|_1 + \lambda_2 \|f\|^2 + \|r\|^2 \\ \text{such that} & K_1 F K_2 + R = S \\ & f \geq 0 \end{array}$$

$F, R =$ matrix form of variables f, r

$K_1,\ K_2$ are linear operators

PDCO solution f is *very sharp*

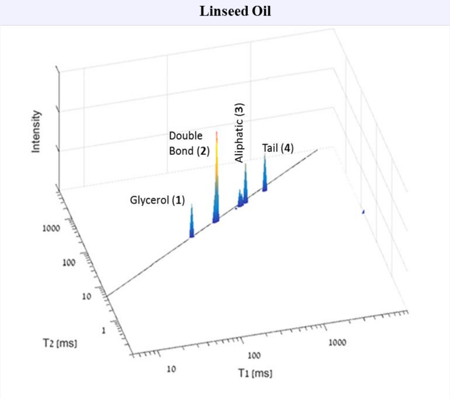


Fig. 4 2D T_1-T_2 ^{1}H LF-NMR energy relaxation spectrum mapping of linseed PUFA oil. (1) Glycerol segment (2) Average of double bonds segment (3) Average of aliphatic middle chain (4) Average of tail segment.

2010s

General-purpose software leads to Applications

- PDCO ideal for signal analysis BPDN, LF-NMR

2010s

General-purpose software leads to Applications

- PDCO ideal for signal analysis BPDN, LF-NMR

Applications lead to new Algorithms

- DQQ procedure for Systems Biology multiscale models — Ding Ma, MS (Stanford)

  Apply MINOS 3 times with and without scaling
  Double-precision, Quad-precision, Quad-precision

2010s

General-purpose software leads to Applications

- PDCO ideal for signal analysis BPDN, LF-NMR

Applications lead to new Algorithms

- DQQ procedure for Systems Biology multiscale models — Ding Ma, MS (Stanford)

  Apply MINOS 3 times with and without scaling
  Double-precision, Quad-precision, Quad-precision

- Algorithm NCL for Taxation policy models — Judd, Ding Ma, Orban, MS

  Nonlinearly Constrained augmented Lagrangian
  New implementation of LANCELOT(using interior methods)

2010s

General-purpose software leads to Applications

- PDCO ideal for signal analysis BPDN, LF-NMR

Applications lead to new Algorithms

- DQQ procedure for Systems Biology multiscale models — Ding Ma, MS (Stanford)

  Apply MINOS 3 times with and without scaling
  Double-precision, Quad-precision, Quad-precision

- Algorithm NCL for Taxation policy models — Judd, Ding Ma, Orban, MS

  Nonlinearly Constrained augmented Lagrangian
  New implementation of LANCELOT(using interior methods)

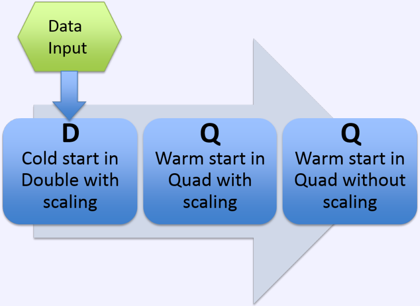
We need general-purpose software to implement the new procedures

DQQ procedure

Ding Ma, MS, . . . (2017)

DQQ procedure

- Multiscale optimization in systems biology
  Double-precision MINOS + Quad-precision MINOS



DQQ procedure

- Multiscale optimization in systems biology
  Double-precision MINOS + Quad-precision MINOS
- Jan 2017 Conference in Oman
  Stop in Paris on the way back . . . !

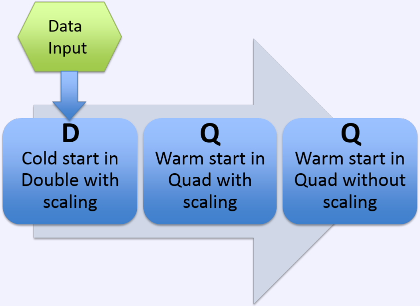


Table: Three large ME biochemical network models TMA_ME, GlcAerWT, GlcAlift. Dimensions of $m \times n$ constraint matrices S, size of the largest optimal primal and dual variables x^*, y^*, number of iterations and runtimes in seconds for each step, and the total runtime of each model.

ME model	TMA_ME	GlcAerWT	GlcAlift
m	18210	68300	69529
n	17535	76664	77893
nnz(S)	336302	926357	928815
$\max \lvert S_{ij} \rvert$	2.1e+04	8.0e+05	2.6e+05
$\lVert x^* \rVert_\infty$	5.9e+00	6.3e+07	6.3e+07
$\lVert y^* \rVert_\infty$	1.1e+00	2.4e+07	2.4e+07
D itns	21026	47718	93857
D time	350.9	10567.8	15913.7
Q1 itns	597	4287	1631
Q1 time	29.0	1958.9	277.3
Q2 itns	0	4	1
Q2 time	5.4	72.1	44.0
Total time	385	12599	16235

Table: Three large ME biochemical network models TMA_ME, GlcAerWT, GlcAlift. Optimal objective value of each step, Pinf and Dinf = final maximum primal and dual infeasibilities ($\log_{10}$ values tabulated, except – means 0). Bold figures show the final *(step Q2)* Pinf and Dinf.

ME model	Step	Objective	Pinf	Dinf
TMA_ME	D	8.3789966820e−07	−06	−05
	Q1	8.7036315385e−07	−25	−32
	Q2	8.7036315385e−07	**–**	−**32**
GlcAerWT	D	−6.7687059922e+05	−04	+00
	Q1	−7.0382449681e+05	−07	−26
	Q2	−7.0382449681e+05	−**21**	−**22**
GlcAlift	D	−5.3319574961e+05	−03	−01
	Q1	−7.0434008750e+05	−08	−22
	Q2	−7.0434008750e+05	−**18**	−**23**

Algorithm NCL

Ken Judd, Ding Ma, Dominique Orban, MS (2018)

Optimal Tax Policy

Kenneth Judd and Che-Lin Su 2011

AMPL model, required a new solver: Algorithm NCL

Optimal tax policy

$$
\begin{array}{llrl}
\text{TAX} & \text{maximize}_{c,\,y} & \sum_i \lambda_i U^i(c_i, y_i) & \\
& \text{subject to} & U^i(c_i, y_i) - U^i(c_j, y_j) \ge 0 & \text{for all } i, j \ (*) \\
& & \lambda^T(y - c) \ge 0 & \\
& & c,\ y \ge 0 &
\end{array}
$$

Optimal tax policy

$$\begin{array}{llrl} \text{TAX} & \text{maximize}_{c,\,y} & \sum_i \lambda_i U^i(c_i, y_i) & \\ & \text{subject to} & U^i(c_i, y_i) - U^i(c_j, y_j) \ge 0 & \text{for all } i, j \ (*) \\ & & \lambda^T(y - c) \ge 0 & \\ & & c,\ y \ge 0 & \end{array}$$

where c_i and y_i are the consumption and income of taxpayer i, and λ is a vector of positive weights. Each utility function $U^i(c_i, y_i)$ has the form

$$U(c, y) = \frac{(c - \alpha)^{1-1/\gamma}}{1 - 1/\gamma} - \psi \frac{(y/w)^{1/\eta+1}}{1/\eta + 1}$$

where w is the wage rate and α, γ, ψ, η are taxpayer heterogeneities

$(*)$ = zillions of incentive-compatibility constraints

Example Tax Problem

TAX	$\underset{x}{\text{minimize}}$	$\varphi(x)$
	subject to	$c(x) \geq 0, \quad \ell \leq x \leq u$

Example: 571000 constraints $c_i(x) \geq 0$, 1500 variables x

10000 constraints $c_i(x^*) \leq 10^{-6}$ (essentially active, LICQ fails)

AMPL model

TAX	$\text{maximize}_{c,\,y}$	$\sum_i \lambda_i U^i(c_i, y_i)$	
	subject to	$U^i(c_i, y_i) - U^i(c_j, y_j) \geq 0$	for all $i \neq j$
		$\lambda^T(y - c) \geq 0$	
		$c,\ y \geq 0$	

```
Incentive{(i,j,k,g,h) in T, (p,q,r,s,t) in T:
          !(i=p and j=q and k=r and g=s and h=t)}:
      (c[i,j,k,g,h] - alpha[k])^(1-1/gamma[h]) / (1-1/gamma[h])
       - psi[g]*(y[i,j,k,g,h]/w[i])^mu1[j] / mu1[j]
    - (c[p,q,r,s,t] - alpha[k])^(1-1/gamma[h]) / (1-1/gamma[h])
       + psi[g]*(y[p,q,r,s,t]/w[i])^mu1[j] / mu1[j]
      >= 0;

Technology:
   sum{(i,j,k,g,h) in T} lambda[i,j,k,g,h]*(y[i,j,k,g,h] - c[i,j,k,g,h]) >= 0;
```

Piecewise-smooth extension

```
Incentive{(i,j,k,g,h) in T, (p,q,r,s,t) in T:
          !(i=p and j=q and k=r and g=s and h=t)}:
   (if c[i,j,k,g,h] - alpha[k] >= epsilon then
      (c[i,j,k,g,h] - alpha[k])^(1-1/gamma[h]) / (1-1/gamma[h])
       - psi[g]*(y[i,j,k,g,h]/w[i])^mu1[j] / mu1[j]
    else
       -  0.5/gamma[h] *epsilon^(-1/gamma[h]-1)*(c[i,j,k,g,h] - alpha[k])^2
       + (1+1/gamma[h])*epsilon^(-1/gamma[h]  )*(c[i,j,k,g,h] - alpha[k])
       + (1/(1-1/gamma[h]) - 1 - 0.5/gamma[h])*epsilon^(1-1/gamma[h])
       - psi[g]*(y[i,j,k,g,h]/w[i])^mu1[j] / mu1[j]
   )
 - (if c[p,q,r,s,t] - alpha[k] >= epsilon then
      ...
   ) >= 0;
```

LANCELOT's BCL algorithm for general NLP

Conn, Gould & Toint (1992)

LANCELOT

$$\boxed{\min \phi(x) \quad \text{st} \quad c(x) = 0, \quad \ell \le x \le u}$$

BCL subproblems (Bound-Constrained augmented Lagrangian):

$$\boxed{\begin{array}{lll} \text{BC}_k & \underset{x}{\text{minimize}} & \phi(x) - y_k^T c(x) + \frac{1}{2}\rho_k c(x)^T c(x) \\ & \text{subject to} & \ell \le x \le u \end{array}}$$

LANCELOT

$$\min \phi(x) \quad \text{st} \quad c(x) = 0, \quad \ell \le x \le u$$

BCL subproblems (Bound-Constrained augmented Lagrangian):

BC_k

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \phi(x) - y_k^T c(x) + \frac{1}{2}\rho_k c(x)^T c(x) \\ \text{subject to} & \ell \le x \le u \end{array}$$

Loop:

solve BC_k to get x_k^*	decreasing opttol ω_k
if $\lVert c(x_k^*)\rVert \le \eta_k$, $y_{k+1} \leftarrow y_k - \rho_k c(x_k^*)$	decreasing featol η_k
else $\quad \rho_{k+1} \leftarrow 10\rho_k$	

LANCELOT

$$\min \phi(x) \quad \text{st} \quad c(x) = 0, \quad \ell \le x \le u$$

BCL subproblems (Bound-Constrained augmented Lagrangian):

$$\text{BC}_k \qquad \underset{x}{\text{minimize}} \quad \phi(x) - y_k^T c(x) + \tfrac{1}{2}\rho_k c(x)^T c(x) \qquad \text{subject to} \quad \ell \le x \le u$$

Loop:

solve BC_k to get x_k^*	decreasing opttol ω_k
if $\|c(x_k^*)\| \le \eta_k$, $y_{k+1} \leftarrow y_k - \rho_k c(x_k^*)$	decreasing featol η_k
else $\rho_{k+1} \leftarrow 10\rho_k$	

Only about 10 subproblems, no LICQ worries

NCL subproblems

$$\text{NLP} \qquad \underset{x}{\text{minimize}} \;\; \phi(x) \qquad \text{subject to} \;\; c(x) = 0, \quad \ell \le x \le u$$

LANCELOT solves about 10 BCL subproblems, causing $c(x) \to 0$:

$$\text{BC}_k \qquad \underset{x}{\text{minimize}} \;\; L(x, y_k, \rho_k) = \phi(x) - y_k^T c(x) + \tfrac{1}{2}\rho_k c(x)^T c(x) \qquad \text{subject to} \;\; \ell \le x \le u$$

NCL subproblems

NLP

$$\underset{x}{\text{minimize}} \quad \phi(x)$$
$$\text{subject to} \quad c(x) = 0, \quad \ell \le x \le u$$

LANCELOT solves about 10 BCL subproblems, causing $c(x) \to 0$:

BC_k

$$\underset{x}{\text{minimize}} \quad L(x, y_k, \rho_k) = \phi(x) - y_k^T c(x) + \tfrac{1}{2}\rho_k c(x)^T c(x)$$
$$\text{subject to} \quad \ell \le x \le u$$

Introduce $r = -c(x)$: $r \to 0$

NC_k

$$\underset{x,\, r}{\text{minimize}} \quad \phi(x) + y_k^T r + \tfrac{1}{2}\rho_k r^T r$$
$$\text{subject to} \quad c(x) + r = 0, \quad \ell \le x \le u$$

Free vars r make the constraints independent and feasible   Interior solvers happy!

NCL subproblems

NLP	$$\underset{x}{\text{minimize}} \quad \phi(x)$$ $$\text{subject to} \quad c(x) = 0, \quad \ell \le x \le u$$

NC_k	$$\underset{x,\,r}{\text{minimize}} \quad \phi(x) + y_k^T r + \tfrac{1}{2}\rho_k r^T r$$ $$\text{subject to} \quad c(x) + r = 0, \quad \ell \le x \le u$$

Free vars r make the constraints independent and feasible   Interior solvers happy!

NCL subproblems for Ken's problem

NLP	$\underset{x}{\text{minimize}} \quad \phi(x)$
	subject to $\quad c(x) \geq 0, \quad \ell \leq x \leq u$

NC_k	$\underset{x,\,r}{\text{minimize}} \quad \phi(x) + y_k^T r + \frac{1}{2}\rho_k r^T r$
	subject to $\quad c(x) + r \geq 0, \quad \ell \leq x \leq u$

Free vars r make the constraints independent and feasible   Interior solvers happy!

LANCELOT on problem TAX (BCL method, 2nd derivs)

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2 \quad m = 32220 \quad n = 360$

k	rhok	omegak	etak	Obj	itns	CGit	TRradius	active
1	1.0e+1	1.0e-1	1.0e-1	-417.455	18	12000	4.1e-01	2831
2	1.0e+1	1.0e-2	1.2e-2	-421.606	39	9000	1.6e-01	2568
3	1.0e+2	1.0e-2	7.9e-2	-421.011	23	11000	2.4e-01	1662
4	1.0e+2	1.0e-4	1.3e-3	-420.188	282	104000	8.6e-02	1444
5	1.0e+3	1.0e-3	6.3e-2	-419.967	134	64000	5.7e-02	1004
6	1.0e+3	1.0e-6	1.3e-4	-419.819	198	156000	3.1e-02	901
7	1.0e+4	1.0e-4	5.0e-2	-419.741	300	308000	3.1e-12	710
8	1.0e+4	1.0e-6	1.3e-5	-419.698	327	623000	5.5e-04	709
9	1.0e+5	1.0e-5	4.0e-2	-419.682	253	724000	4.7e-03	653
10	1.0e+5	1.0e-6	1.3e-6	-419.676	154	1031000	4.2e-11	663
11	1.0e+6	1.0e-6	3.2e-2	...				

1970 iterations, 8 hours CPU on NEOS

(SNOPT and IPOPT fail)

NCL/IPOPT on problem TAX

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2 \quad m = 32220 \quad n = 360$

k	ρ_k	η_k	$\|r_k^*\|_\infty$	$\phi(x_k^*)$	mu_init	Itns	Time
1	10^2	10^{-2}	7.0e-03	-4.2038075e+02	10^{-1}	95	40.8
2	10^2	10^{-3}	4.1e-03	-4.2002898e+02	10^{-4}	17	7.0
3	10^3	10^{-3}	1.3e-03	-4.1986069e+02	10^{-4}	20	8.5
4	10^4	10^{-3}	4.4e-04	-4.1972958e+02	10^{-5}	57	32.6
5	10^4	10^{-4}	2.2e-04	-4.1968646e+02	10^{-5}	29	14.6
6	10^5	10^{-4}	9.8e-05	-4.1967560e+02	10^{-6}	36	18.7
7	10^5	10^{-5}	3.9e-05	-4.1967205e+02	10^{-6}	35	19.7
8	10^6	10^{-5}	4.2e-06	-4.1967150e+02	10^{-7}	18	7.7
9	10^6	10^{-6}	9.4e-07	-4.1967138e+02	10^{-7}	15	6.8

322 iterations, 3 mins CPU

NCL/IPOPT bigger example

$na, nb, nc, nd, ne = 21, 3, 3, 2, 2 \quad m = 570780 \quad n = 1512$

k	ρ_k	η_k	$\|r_k^*\|_\infty$	$\phi(x_k^*)$	mu_init	Itns	Time
1	10^2	10^{-2}	5.1e-03	-1.7656816e+03	10^{-1}	825	7763
2	10^2	10^{-3}	2.4e-03	-1.7648480e+03	10^{-4}	66	473
3	10^3	10^{-3}	1.3e-03	-1.7644006e+03	10^{-4}	106	771
4	10^4	10^{-3}	3.8e-04	-1.7639491e+03	10^{-5}	132	1347
5	10^4	10^{-4}	3.2e-04	-1.7637742e+03	10^{-5}	229	2451
6	10^5	10^{-4}	8.6e-05	-1.7636804e+03	10^{-6}	104	1097
7	10^5	10^{-5}	4.9e-05	-1.7636469e+03	10^{-6}	143	1633
8	10^6	10^{-5}	1.5e-05	-1.7636252e+03	10^{-7}	71	786
9	10^7	10^{-5}	2.8e-06	-1.7636196e+03	10^{-7}	67	726
10	10^7	10^{-6}	5.1e-07	-1.7636187e+03	10^{-8}	18	171

1761 iterations, 5 hours CPU

Warm-start options for Nonlinear Interior Methods

IPOPT	warm_start_init_point=yes	
	mu_init=1e-4	(1e-5, ..., 1e-8)
KNITRO	algorithm=1	Thanks, Richard Waltz!
	bar_directinterval=0	
	bar_initpt=2	
	bar_murule=1	
	bar_initmu=1e-4	(1e-5, ..., 1e-8)
	bar_slackboundpush=1e-4	(1e-5, ..., 1e-8)

NCL/KNITRO with Warm Starts

na = increasing $nb = 3$ $nc = 3$ $nd = 2$ $ne = 2$

			IPOPT		KNITRO		NCL/IPOPT		NCL/KNITRO	
na	m	n	itns	time	itns	time	itns	time	itns	time
5	32220	360	449	217	168	53	322	146	339	63
9	104652	648	> 98*	> 360*	928	825	655	1023	307	239
11	156420	792	> 87*	∞!	2769	4117	727	1679	383	420
17	373933	1224			2598	11447	1021	6347	486	1200
21	570780	1512					1761	17218	712	2880

Warm starts Warm starts

Summary

General-Purpose Software

We couldn't guess the earlier applications of optimization!

Existing software $\rightarrow$ New applications

MINOS	Energy/economic models
NPSOL	trajectory optimization, radiation therapy
SNOPT	trajectory optimization (bigger), shape optimization, robotics
PDCO	Basis Pursuit Denoising (signal analysis), LF-NMR analysis

General-Purpose Software

We couldn't guess the earlier applications of optimization!

Existing software → New applications

MINOS	Energy/economic models
NPSOL	trajectory optimization, radiation therapy
SNOPT	trajectory optimization (bigger), shape optimization, robotics
PDCO	Basis Pursuit Denoising (signal analysis), LF-NMR analysis

New applications → New algorithms to help existing software

Systems biology (multiscale)	DQQ: combine DoubleMINOS + QuadMINOS
Taxation policy	NCL: seq of subproblems, warm-start IPOPT, KNITRO

General-Purpose Software

We couldn't guess the earlier applications of optimization!

Existing software → New applications

MINOS	Energy/economic models
NPSOL	trajectory optimization, radiation therapy
SNOPT	trajectory optimization (bigger), shape optimization, robotics
PDCO	Basis Pursuit Denoising (signal analysis), LF-NMR analysis

New applications → New algorithms to help existing software

Systems biology (multiscale)	DQQ: combine DoubleMINOS + QuadMINOS
Taxation policy	NCL: seq of subproblems, warm-start IPOPT, KNITRO
Hamiltonian cycles in graphs (2018: Ali Eshragh, Australia)	MINOS simplex method: change 1 subroutine

2020s

2020s (Now and the Future)

- Autonomous vehicles
  Smooth path, failsafe
  Chris Maes (ICME, NVidia)

2020s (Now and the Future)

- Autonomous vehicles
  Smooth path, failsafe
  Chris Maes (ICME, NVidia)

- Xing Lab @ Stanford
  AI, physics, engineering, biology, medicine
  Diagnosis, treatment planning, nanotech imaging for precision medicine

2020s (Now and the Future)

- Autonomous vehicles
  Smooth path, failsafe
  Chris Maes (ICME, NVidia)

- Xing Lab @ Stanford
  AI, physics, engineering, biology, medicine
  Diagnosis, treatment planning, nanotech imaging for precision medicine

- 1998– Gamma-Knife radiation therapy
  NPSOL used for many years in Sweden — Body moves during radiation

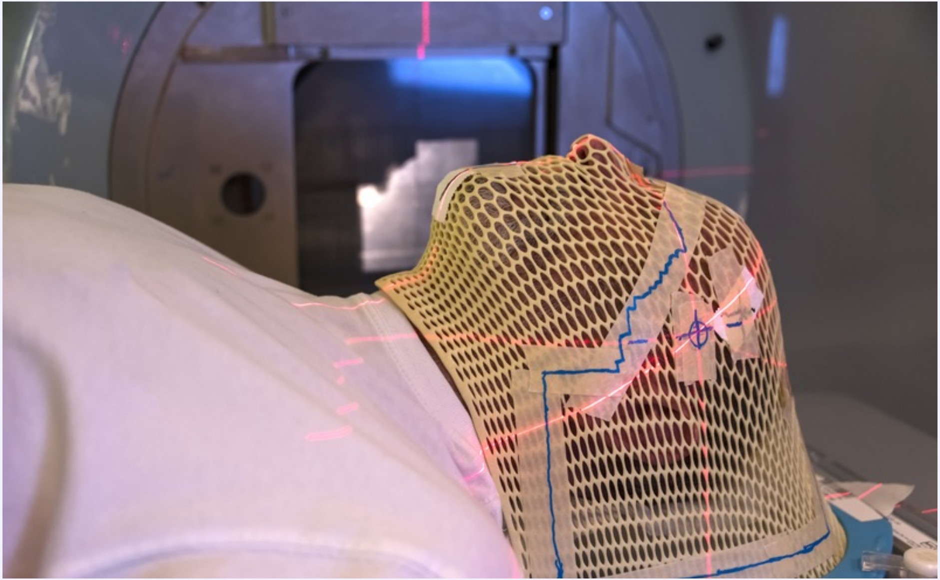
2020s (Now and the Future)

- Autonomous vehicles
  Smooth path, failsafe
  Chris Maes (ICME, NVidia)

- Xing Lab @ Stanford
  AI, physics, engineering, biology, medicine
  Diagnosis, treatment planning, nanotech imaging for precision medicine

- 1998– Gamma-Knife radiation therapy
  NPSOL used for many years in Sweden — Body moves during radiation
- 2018– FLASH radiotherapy (Billy Loo, Sami Tantawi @ SLAC, Stanford)
  X-rays or protons — Only 1 second of radiation

Flash Radiotherapy



Optimization

Stabilize aircraft

Minimize fuel

Reduce CO_2

Make the world a better place

Special thanks

SOL	**George Dantzig, Richard Cottle**
Algorithm coauthors	Philip Gill, Walter Murray, Bruce Murtagh
Software coauthors	Philip Gill, Elizabeth Wong (UCSD)

Special thanks

SOL	**George Dantzig, Richard Cottle**
Algorithm coauthors	Philip Gill, Walter Murray, Bruce Murtagh
Software coauthors	Philip Gill, Elizabeth Wong (UCSD)
PDCO applications	
Basis Pursuit Denoising	Shaobing Chen, David Donoho (Stanford)
LF-NMR	Ofer Levi, Shirley Berman, Zeev Wiesman (Israel)

Special thanks

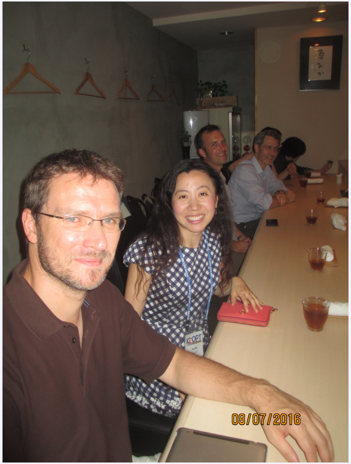
SOL	**George Dantzig, Richard Cottle**
Algorithm coauthors	Philip Gill, Walter Murray, Bruce Murtagh
Software coauthors	Philip Gill, Elizabeth Wong (UCSD)
PDCO applications	
Basis Pursuit Denoising	Shaobing Chen, David Donoho (Stanford)
LF-NMR	Ofer Levi, Shirley Berman, Zeev Wiesman (Israel)
DQQ	Ding Ma, MS, Ronan Fleming, Ines Thiele (2017)
NCL	Ding Ma, MS, Ken Judd, Dominique Orban (2018)

Special thanks

SOL	**George Dantzig, Richard Cottle**
Algorithm coauthors	Philip Gill, Walter Murray, Bruce Murtagh
Software coauthors	Philip Gill, Elizabeth Wong (UCSD)
PDCO applications	
Basis Pursuit Denoising	Shaobing Chen, David Donoho (Stanford)
LF-NMR	Ofer Levi, Shirley Berman, Zeev Wiesman (Israel)
DQQ	Ding Ma, MS, Ronan Fleming, Ines Thiele (2017)
NCL	Ding Ma, MS, Ken Judd, Dominique Orban (2018)
LANCELOT	Conn, Gould, and Toint (1992)
BCL, LCL	Michael Friedlander (MS&E 2002)
AMPL, IPOPT, KNITRO	Fourer & Gay, Biegler & Wachter, Waltz

Special thanks (NCL)

Ken, Che-Lin, Dominique/Ding/Michael



Special thanks (while working)

Yuja Wang, YouTube (and YouKu!)

Special thanks (DQQ and NCL)

IEEM2023 Conference, Marina Bay Sands, Singapore, Dec 18–21, 2023

Ding and daughter Emma