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

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SOL
Systems Optimization Laboratory

George Dantzig, Stanford University, 1974
Inventor of the Simplex Method
Father of linear programming

Large-scale optimization:
Algorithms, software, applications

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, MINOS first version
1979–87	Philip Gill, Walter Murray, MS, Margaret Wright (Gang of 4!)
1989–	Gerd Infanger, stochastic optimization
1979–	Walter Murray, MS, many students
2002–	Yinyu Ye, optimization algorithms, especially interior methods
This week!	UC Berkeley opened George B. Dantzig Auditorium

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**	

1970s

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)

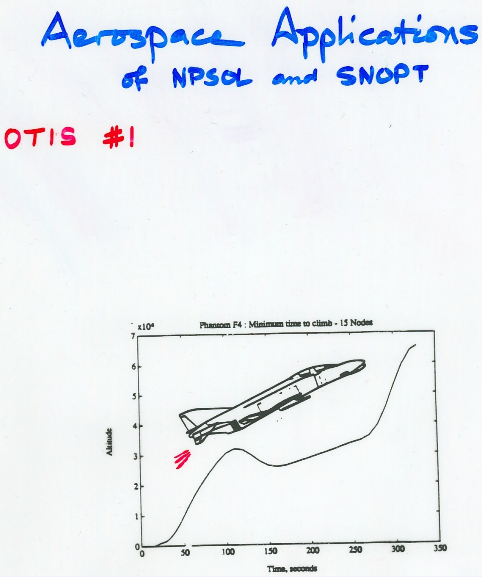
- Optimal Power Flow @ General Electric
- Aerospace optimization @ NASA, McDonnell-Douglas

1990s

1990s

- Alan Manne: MERGE greenhouse-gas model (sparse nonlinear constraints)
- Philip Gill: Aerospace trajectory optimization @ McDonnell-Douglas

F-4	Minimum time-to-climb
DC-Y SSTO	Minimum-fuel landing maneuver



Start at sea-level

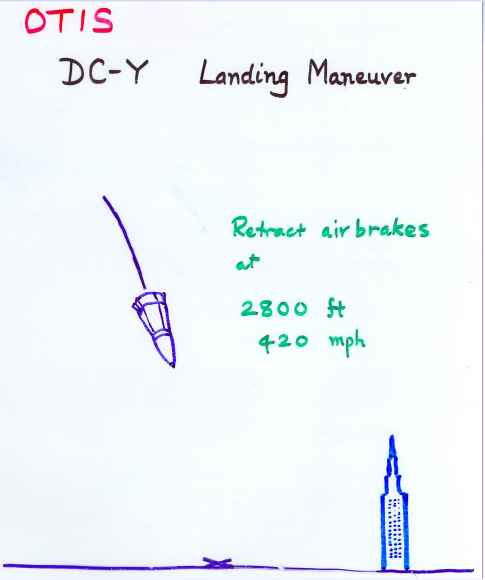
Climb to 20,000m
Speed Mach 1

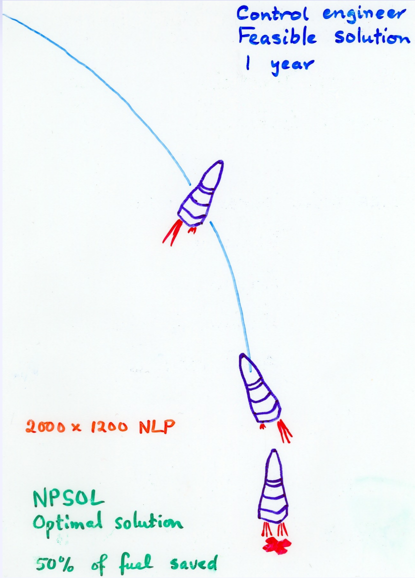
DC-X single-stage-to-orbit prototype

1/3 full-size = 13m tall

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

← Taking-off?
Landing?


OTIS
DC-Y Landing Maneuver
Retract air brakes
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 = 900m
- 2nd optimization: starting altitude = variable

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- New constraint needed:

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Optimum starting altitude = 450m(!)

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Optimum starting altitude = 450m(!)

Come back Alan Shephard!

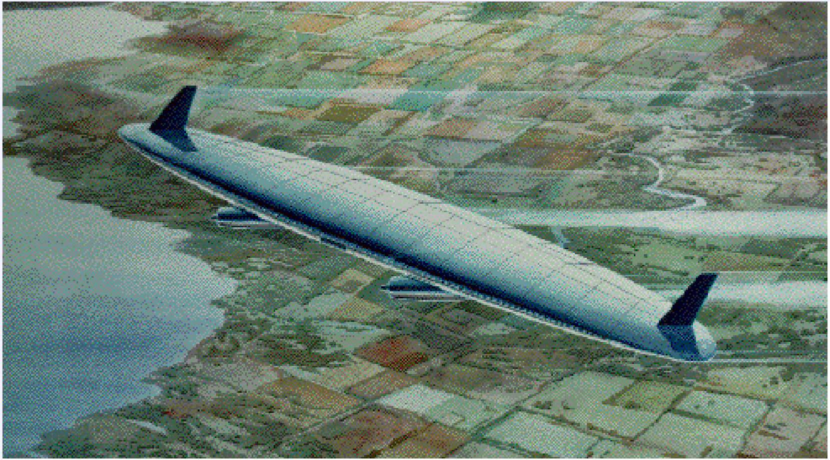
2000s

2000s

David Saunders, NASA Ames (Calif)

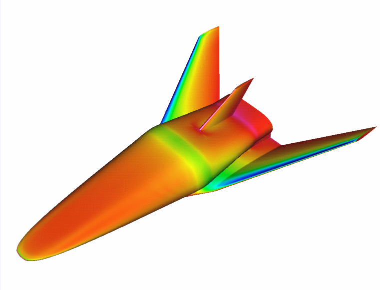
- Wǒ shuāng bāotāi!
  1970: visit Stanford for 1 month
  (now 49 years)
- Shape optimization
  Supersonic airliners
- Trajectory optimization
  SHARP (next Space Shuttle)

OAW oblique all-wing airliner



HSCT high speed civil transport

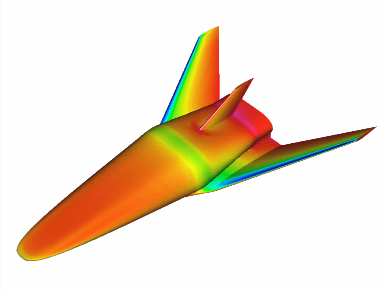
CTV crew transfer vehicle



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



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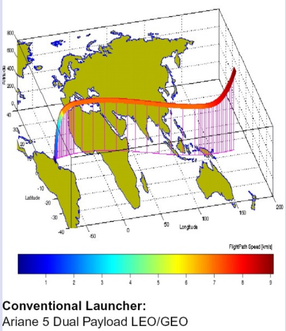
- Trajectory optimization with SNOPT
- Could always abort to Kennedy, Boston, Gander, or Shannon
- 4000-mile cross-range capability during reentry

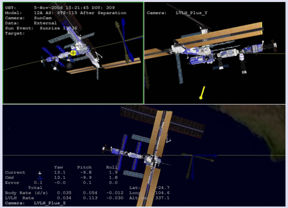
Image credit: David Kinney, NASA Ames Research Center

SNOPT Applications

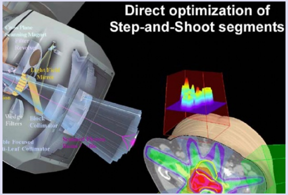
Trajectory optimization
Launch 2 satellites



Manoeuver ISS
Space Station



Torque minimization
Robot at JPL
Daniel Clemente



Radiation therapy
Control problem
Paul Keall

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)

- Tried shape optimization of heat shield and shoulder curvature (but the Apollo folk were pretty close already)

Stratolaunch carrier aircraft (first flight April 15)

AIAA 2018

Stratolaunch carrier aircraft (first flight April 15)

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

Signal analysis using PDCO

Primal-Dual interior method for Convex Objective

General-purpose MATLAB software

$$\min \ \varphi(x) \ \text{ st } \ Ax = b, \ \ \ell \le x \le u$$

Unique feature: A may be an operator

Iterative method LSMR computes each search direction

Signal analysis using PDCO

Primal-Dual interior method for Convex Objective

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$$\min\ \varphi(x) \quad \text{st} \quad Ax = b, \quad \ell \le x \le u$$

Unique feature: A may be an operator

Iterative method LSMR computes each search direction

- 1998 BPDN: Basis Pursuit DeNoising — Shaobing Chen, David Donoho, MS (Stanford)
- 2011 1D LF-NMR (Low-Field NMR analysis) — Ofer Levi, MS, Berman, Wiesman, . . . (Israel)
- 2018 2D LF-NMR

2D LF-NMR analysis using PDCO

Linseed Oil

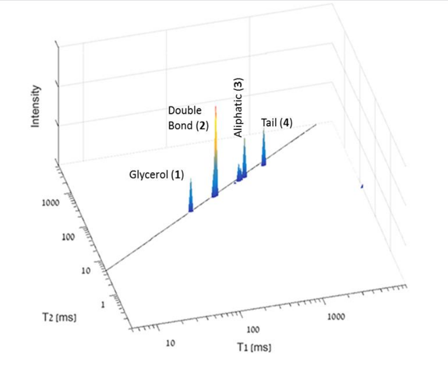

Fig. 4 2D T_1-T_2 ^{1}H LF-NMR energy relaxation spectrum mapping of linseed PUFA oil.

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

PDCO solution f is *very sharp*

2010s

General-purpose software leads to Applications

- PDCO ideal for LF-NMR analysis

Applications lead to Algorithms

- Systems Biology multiscale models lead to DQQ procedure — Ding Ma, MS (Stanford)
- Taxation policy models lead to NCL procedure — Ding Ma, MS, Judd, Orban
- Need general-purpose software to implement new procedures

2010s

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- Need general-purpose software to implement new procedures

DQQ = Double-precision / Quad-precision / Quad-precision solvers

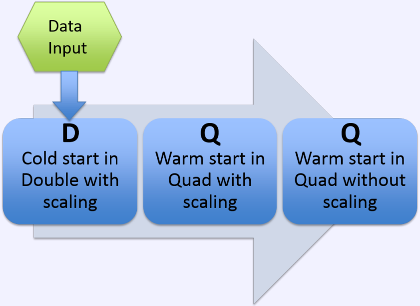
cold start / warm start / warm start

NCL = Nonlinearly Constrained augmented Lagrangian

need interior methods

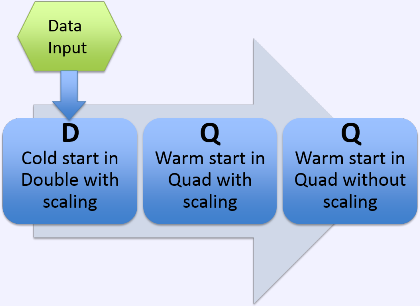
DQQ procedure (Ding Ma, MS, . . .)

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



DQQ procedure (Ding Ma, MS, . . .)

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



NCL procedure (Ding Ma, MS, . . .)

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

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

10000 constraints $c_i(x^*) \le 10^{-6}$ (essentially active)

NCL procedure (Ding Ma, MS, ...)

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NCL procedure $\approx$ 10 easier subproblems, updating y_k or increasing ρ_k:

NC_k	$\displaystyle\min_{x,\,r} \ \phi(x) + y_k^T r + \tfrac{1}{2}\rho_k \|r\|^2$ subject to $c(x) + r \ge 0, \quad \ell \le x \le u$

NCL procedure (Ding Ma, MS, . . .)

Taxation problem

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

Example: 571000 constraints $c_i(x) \ge 0$, 1500 variables x
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NCL procedure $\approx$ 10 easier subproblems, updating y_k or increasing ρ_k:

NC_k

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

- Variables r make the nonlinear constraints independent and feasible
- Interior solvers IPOPT, KNITRO happy as $r \to 0$

Summary

General-Purpose Software

We couldn't guess the earlier applications of optimization!

Existing software → New applications 1980–now

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

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New applications → New algorithms to help existing software 2010s: Ding Ma, ...

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

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Existing software → Prototype new applications 2018: Ali Eshragh, . . . (Australia)

MINOS Find Hamiltonian cycles in graphs
Add one subroutine to MINOS simplex method

2020s

2020s

Now and future:

- Autonomous vehicles
  Smooth path, failsafe

2020s

Now and future:

- Autonomous vehicles
  Smooth path, failsafe
- Xing Lab @ Stanford
  AI, physics, engineering, biology in medicine
  Diagnosis, treatment planning, nanotech imaging for precision medicine

2020s

Now and future:

- Autonomous vehicles
  Smooth path, failsafe
- Xing Lab @ Stanford
  AI, physics, engineering, biology in medicine
  Diagnosis, treatment planning, nanotech imaging for precision medicine
- 1998 Radiation therapy
  NPSOL: Gamma-Knife Body moves during radiation

2020s

Now and future:

- Autonomous vehicles
  Smooth path, failsafe
- Xing Lab @ Stanford
  AI, physics, engineering, biology in medicine
  Diagnosis, treatment planning, nanotech imaging for precision medicine
- 1998 Radiation therapy
  NPSOL: Gamma-Knife — Body moves during radiation
- 2018 Billy Loo, Sami Tantawi @ SLAC (Stanford)
  FLASH therapy (X-rays or protons) — Only 1 second of radiation


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
Software coauthors	Bruce Murtagh, Philip Gill, Elizabeth Wong
Basis Pursuit	Shaobing Chen, David Donoho
LF-NMR	Ofer Levi, Shirley Berman, Zeev Wiesman, . . .
DQQ	Ding Ma, Ronan Fleming, Ines Thiele
NCL	Ding Ma, Ken Judd, Dominique Orban
AMPL, IPOPT, KNITRO	developers

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NCL	Ding Ma, Ken Judd, Dominique Orban
AMPL, IPOPT, KNITRO	developers
AI+IoT organizers	**Markla, New Fortune**
YouTube, Youku	**Yuja Wang**

YouTube companion Yuja Wang

Liǎng gè Yōukù péngyǒu Láng Lǎng hé Wáng Yǔjiā

Two equally amazing stars (optimal!)