PRIMA: What, Why, How, and So What?

Zaikun Zhang

The Hong Kong Polytechnic University

ICIAM 2023, Tokyo, Japan

What is this talk about?

Derivative-Free Optimization (DFO):

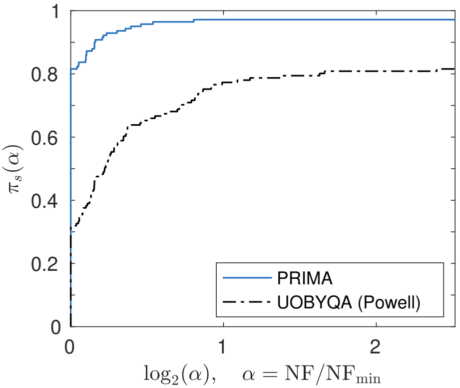
Optimization without using derivatives

Topics of this talk:

1. A new DFO solver named PRIMA
2. The mathematics behind it

Let us start with some tests of PRIMA based on the CUTEst problems.

Performance of PRIMA compared with Powell's solvers



PRIMA v.s. UOBYQA

(unconstrained problems, at most 100 variables)

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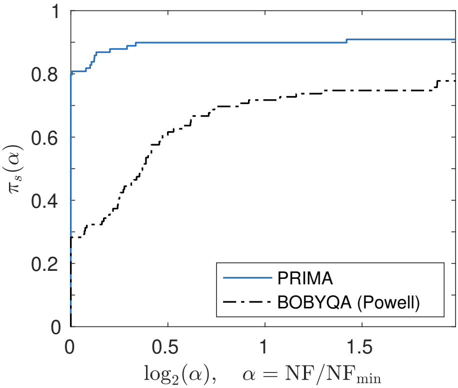
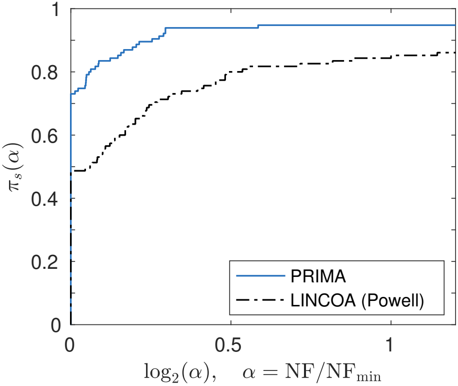


PRIMA v.s. BOBYQA

(bound-constrained problems, at most 200 variables)

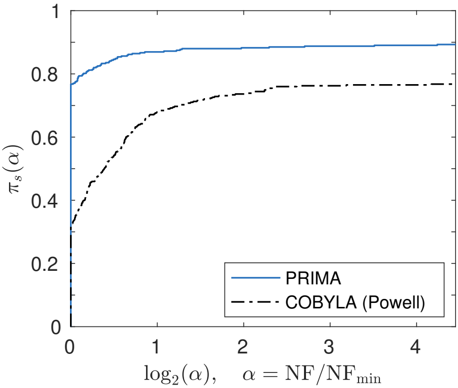
Performance of PRIMA compared with Powell's solvers



PRIMA v.s. LINCOA

(linearly constrained problems, at most 200 variables, 20,000 constraints)

Performance of PRIMA compared with Powell's solvers



PRIMA v.s. COBYLA

(nonlinearly constrained problems, at most 100 variables, 10,000 constraints)

Sorry, I lied ...

Topics of this talk:

1. ~~A new DFO solver named PRIMA~~

   PRIMA is not a new solver but a re-implementation of Powell's solvers.

2. ~~The mathematics behind it~~

   There is no mathematics in this talk.

PRIMA: Reference Implementation for Powell's Methods with Modernization and Amelioration

Zaikun Zhang

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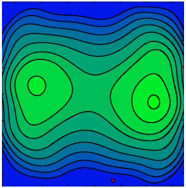
Dedicated to the late Professor **M. J. D. Powell** FRS (1936–2015)

Funding: Hong Kong RGC grants 253012/17P, 153054/20P, and 153066/21P.

Trust-region DFO methods based on interpolation models



$$x_{k+1} \approx x_k + \underset{\|d\| \le \Delta_k}{\arg\min}\, M_k(x_k + d)$$

- M_k is the trust-region model (surrogate)
  - $M_k(x) \approx f(x)$ around x_k
  - M_k interpolates f on a set $\mathcal{X}_k$ consisting of previous iterates
- $\|d\| \le \Delta_k$ is the trust-region constraint
  - If "things work well", increase Δ_k
  - Otherwise, decrease Δ_k

Images by Dr. F. V. Berghen from `http://www.applied-mathematics.net`.

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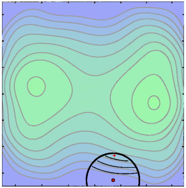

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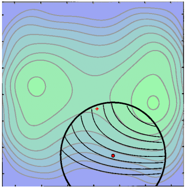

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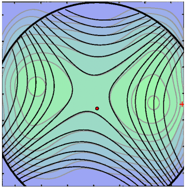

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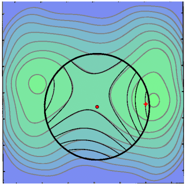

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Maintenance of the interpolation set

The interpolation set $\mathcal{X}_k$ must be updated with care.

- $\mathcal{X}_k$ must reuse previous iterates as much as possible.
- The geometry of $\mathcal{X}_k$ must ensure the well-conditioning of the problem

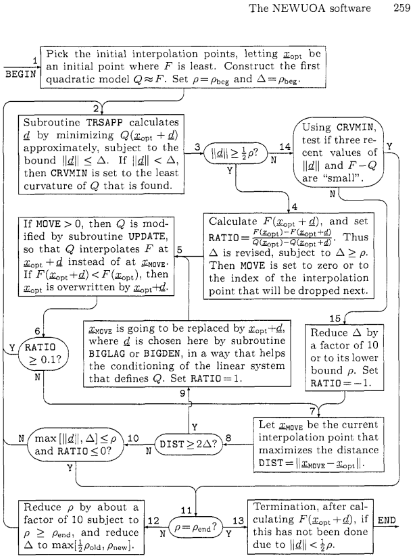
$$M_k(x) = f(x), \quad x \in \mathcal{X}_k.$$

- Normally, $\mathcal{X}_{k+1} = (\mathcal{X}_k \cup \{x_{k+1}\}) \setminus \{\text{a "bad" point}\}$.
- Take geometry-improving steps if the geometry of $\mathcal{X}_k$ deteriorates.

Powell's trust-region DFO algorithms and software

- COBYLA: solving general nonlinearly constrained problems using linear models; code released in 1992; paper published in 1994
- UOBYQA: solving unconstrained problems using quadratic models; code released in 2000; paper published in 2002
- NEWUOA: solving unconstrained problems using quadratic models; code released in 2004; paper published in 2006
- BOBYQA: solving bound-constrained problems using quadratic models; code released and paper written in 2009
- LINCOA: solving linearly constrained problems using quadratic models; code released in 2013 but no paper written

What do these algorithms look like?



NEWUOA

Implementation of these methods is HARD

> The development of NEWUOA has taken nearly three years. The work was very frustrating ...

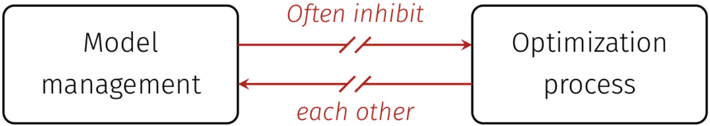
— M. J. D. Powell

The NEWUOA software for unconstrained optimization without derivatives, 2006

N.B.

- NEWUOA was Powell's third trust-region DFO solver, COBYLA and UOBYQA being the first two.
- Mathematically speaking, NEWUOA and UOBYQA are essentially the same except for the ways they construct the model.
- Given the experience with UOBYQA (and COBYLA), Powell still spent three frustrating years on the development of NEWUOA.

The central difficulty



Powell's implementation

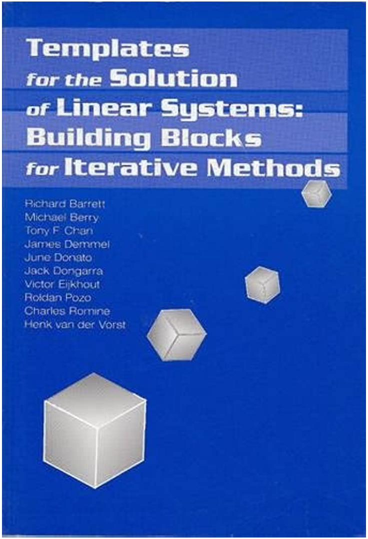
- Powell implemented these five methods into publicly available solvers.
- The solvers are widely used by scientists and engineers.
- They are often used as benchmarks when designing new algorithms.
- However, the implementation was in Fortran 77, with plenty of GOTOs: in total, 7939 lines of code with 249 GOTOs!

A modernized implementation is greatly needed.

Why should I work on a modernized implementation

- Professor Powell, April 2015: "It would be a relief to me if you would kindly continue to look after my optimisation software (NEWUOA, BOBYQA and LINCOA). Also I would like you to add COBYLA and TOLMIN if you do not have them already."
- Stefan Wild, ICCOPT 2016, Tokyo: People do not want interfaces. They want implementations that they can understand and play with.
- Jeff Larson, ISMP 2018, Bordeaux: Numerical linear algebra people have standard implementations for standard algorithms, e.g., LAPACK, whereas we all work on our own implementation of interpolation, model improvement, ...

An inspiration



Isn't it a perfect project for an engineer or a student?

- Given that Powell spent three frustrating years on the development of his own algorithm NEWUOA despite his abundant experience, where could I find this genius engineer who can learn all the five algorithms from scratch and implement them in a reasonable amount of time?
- Assume that I am lucky to find the abovementioned genius engineer and he/she happens to be my Ph.D. student. How should I persuade him/her to be fully devoted to a project for three years (as I did) without producing a single publication? Am I even allowed to do so?

libprima.net

PRIMA is an acronym for

"Reference Implementation for Powell's Methods
with Modernization and Amelioration",

"P" for Powell.

An overview of PRIMA

- The solvers are implemented in a structured and modularized way so that they are understandable, maintainable, extendable, fault-tolerant, and future-proof.
- The code has no GOTO and uses matrix-vector procedures instead of loops whenever possible.
- The implementation is mathematically equivalent to Powell's except for the bug fixes and improvements we introduce intentionally.
- The implementation of PRIMA in modern Fortran (F2008 or above) has been finished.
- Versions in MATLAB, Python, Julia, R, ... will be implemented using the modern Fortran as a reference.
- A MATLAB interface is provided to use the modern Fortran version.
- The inclusion of PRIMA into SciPy is under discussion, and the major SciPy maintainers are positive about it.

Why do I start with modern Fortran?

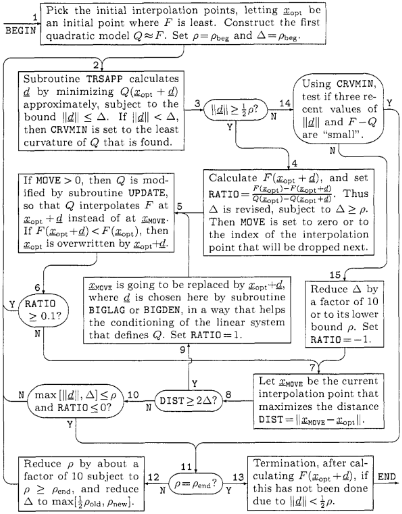
Fortran? Are you a caveman?

- The syntax and style of modern Fortran are very similar to MATLAB.
- I start with modern Fortran, so that I can systematically verify the bit-to-bit faithfulness of PRIMA, as the original code is Fortran.
- With other languages, the verification is hard, if not impossible.

Ultimate goal of PRIMA:
Make Powell's methods available to everyone in her/his favorite languages.

Powell's description of NEWUOA (recapped)

The NEWUOA software 259



NEWUOA

The original implementation of NEWUOA: a snippet

```
  100 KNEW=0
      CALL TRSAPP (N,NPT,XOPT,XPT,GQ,HQ,PQ,DELTA,D,W,W(NP),
     1  W(NP+N),W(NP+2*N),CRVMIN)
      DSQ=ZERO
      DO 110 I=1,N
  110 DSQ=DSQ+D(I)**2
      DNORM=DMIN1(DELTA,DSQRT(DSQ))
      IF (DNORM .LT. HALF*RHO) THEN
          KNEW=-1
          DELTA=TENTH*DELTA
          RATIO=-1.0D0
          IF (DELTA .LE. 1.5D0*RHO) DELTA=RHO
          IF (NF .LE. NFSAV+2) GOTO 460
          TEMP=0.125D0*CRVMIN*RHO*RHO
          IF (TEMP .LE. DMAX1(DIFFA,DIFFB,DIFFC)) GOTO 460
          GOTO 490
      END IF

  120 IF (DSQ .LE. 1.0D-3*XOPTSQ) THEN
          TEMPQ=0.25D0*XOPTSQ
          DO 140 K=1,NPT
          SUM=ZERO
          DO 130 I=1,N
  130     SUM=SUM+XPT(K,I)*XOPT(I)
          TEMP=PQ(K)*SUM
          SUM=SUM-HALF*XOPTSQ
          W(NPT+K)=SUM
          DO 140 I=1,N
          GQ(I)=GQ(I)+TEMP*XPT(K,I)
          XPT(K,I)=XPT(K,I)-HALF*XOPT(I)
          VLAG(I)=BMAT(K,I)
          W(I)=SUM*XPT(K,I)+TEMPQ*XOPT(I)
          IP=NPT+I
          DO 140 J=1,I
  140     BMAT(IP,J)=BMAT(IP,J)+VLAG(I)*W(J)+W(I)*VLAG(J)
```

Faithful pseudocode of NEWUOA in PRIMA

Pick $\mathcal{X} \subset \mathbb{R}^n$ and $\rho > 0$. Let M interpolate f on $\mathcal{X}$. $x_{\text{o}} := \arg\min_{x \in \mathcal{X}} f(x)$. $\Delta := \rho$.

while not converged **do**
    Calculate a trust-region trial point $x_{\text{tr}} \approx \arg\min\{M(x) : \|x - x_{\text{o}}\| \le \Delta\}$
    if $M(x_{\text{o}}) - M(x_{\text{tr}})$ is too small or $\|x_{\text{tr}} - x_{\text{o}}\|$ is too short **then**
        Reduce Δ subject to $\Delta \ge \rho$
    else
        Evaluate the reduction ratio and update Δ accordingly subject to $\Delta \ge \rho$
        if it is proper to replace a point $x_{\text{drop}} \in \mathcal{X}$ with x_{tr} **then**
            Set $\mathcal{X} = \left(\mathcal{X} \cup \{x_{\text{tr}}\}\right) \setminus \{x_{\text{drop}}\}$, and then update M and x_{o}
        end if
    end if
    `improve_geo` := x_{tr} is bad & the geometry of $\mathcal{X}$ is inadequate
    `reduce_rho` := x_{tr} is bad & the geometry of $\mathcal{X}$ is adequate & Δ is small
    if `improve_geo` **then**
        Decide a point $x_{\text{drop}} \in \mathcal{X}$ to drop and a geometry-improving point x_{geo}
        Set $\mathcal{X} = \left(\mathcal{X} \setminus \{x_{\text{drop}}\}\right) \cup \{x_{\text{geo}}\}$, and then update M and x_{o}
    end if
    if `reduce_rho` **then** reduce ρ and reduce Δ subject to $\Delta \ge \rho$
end while

N.B.: The updates keep M interpolating f on $\mathcal{X}$ and $x_{\text{o}} = \arg\min_{x \in \mathcal{X}} f(x)$.

PRIMA NEWUOA: trust-region phase (ln. 2–10)

```fortran

do tr = 1, maxtr
    call trsapp(delta, gopt, hq, pq, trtol, xpt, crvmin, d)
    dnorm = min(delta, norm(d))
    shortd = (dnorm < HALF * rho)
    qred = -quadinc(d, xpt, gopt, pq, hq)

    if (shortd .or. .not. qred > 0) then
        delta = TENTH * delta
        if (delta <= gamma3 * rho) then
            delta = rho  ! Set DELTA to RHO when it is close to or below.
        end if
    else
        x = xbase + (xpt(:, kopt) + d)
        call evaluate(calfun, x, f)
        nf = nf + 1

        dnorm_rec = [dnorm_rec(2:size(dnorm_rec)), dnorm]
        moderr = f - fval(kopt) + qred
        moderr_rec = [moderr_rec(2:size(moderr_rec)), moderr]

        ratio = redrat(fval(kopt) - f, qred, eta1)
        delta = trrad(delta, dnorm, eta1, eta2, gamma1, gamma2, ratio)
        if (delta <= gamma3 * rho) then
            delta = rho  ! Set DELTA to RHO when it is close to or below.
        end if

        ximproved = (f < fval(kopt))
        knew_tr = setdrop_tr(idz, kopt, ximproved, bmat, d, delta, rho, xpt, zmat)
        if (knew_tr > 0) then
            xdrop = xpt(:, knew_tr)
            xosav = xpt(:, kopt)
            call updateh(knew_tr, kopt, d, xpt, idz, bmat, zmat)
            call updatexf(knew_tr, ximproved, f, xosav + d, kopt, fval, xpt)
            call updateq(idz, knew_tr, ximproved, bmat, d, moderr, xdrop, xosav, xpt, zmat, gopt, hq, pq)
            call tryqalt(idz, bmat, fval - fval(kopt), ratio, xpt(:, kopt), xpt, zmat, itest, gopt, hq, pq)
        end if
    end if  ! End of IF (SHORTD .OR. .NOT. QRED > 0). The normal trust-region calculation ends here.

```

PRIMA NEWUOA: `improve_geo`, `reduce_rho` (ln. 11, 12)

```
accurate_mod = all(abs(moderr_rec) <= 0.125 * crvmin * rho**2) .and. all(dnorm_rec <= rho)
distsq = sum((xpt - spread(xpt(:, kopt), dim=2, ncopies=npt))**2, dim=1)
close_itpset = all(distsq <= 4.0 * delta**2)
adequate_geo = (shortd .and. accurate_mod) .or. close_itpset
small_trrad = (max(delta, dnorm) <= rho)
bad_trstep = (shortd .or. (.not. qred > 0) .or. ratio <= eta1 .or. knew_tr == 0)
improve_geo = bad_trstep .and. .not. adequate_geo
bad_trstep = (shortd .or. (.not. qred > 0) .or. ratio <= 0 .or. knew_tr == 0)
reduce_rho = bad_trstep .and. adequate_geo .and. small_trrad
```

PRIMA NEWUOA: post-processing phase (ln. 13–17)

```fortran

    if (improve_geo) then
        knew_geo = int(maxloc(distsq, dim=1), kind(knew_geo))
        delbar = max(min(TENTH * sqrt(maxval(distsq)), HALF * delta), rho)
        d = geostep(idz, knew_geo, kopt, bmat, delbar, xpt, zmat)
        x = xbase + (xpt(:, kopt) + d)
        call evaluate(calfun, x, f)
        nf = nf + 1

        dnorm = min(delbar, norm(d))
        dnorm_rec = [dnorm_rec(2:size(dnorm_rec)), dnorm]
        moderr = f - fval(kopt) - quadinc(d, xpt, gopt, pq, hq)
        moderr_rec = [moderr_rec(2:size(moderr_rec)), moderr]

        ximproved = (f < fval(kopt))
        xdrop = xpt(:, knew_geo)
        xosav = xpt(:, kopt)
        call updateh(knew_geo, kopt, d, xpt, idz, bmat, zmat)
        call updatexf(knew_geo, ximproved, f, xosav + d, kopt, fval, xpt)
        call updateq(idz, knew_geo, ximproved, bmat, d, moderr, xdrop, xosav, xpt, zmat, gopt, hq, pq)
    end if  ! End of IF (IMPROVE_GEO). The procedure of improving geometry ends.

    if (reduce_rho) then
        if (rho <= rhoend) then
            info = SMALL_TR_RADIUS
            exit
        end if
        delta = HALF * rho
        rho = redrho(rho, rhoend)
        delta = max(delta, rho)
        dnorm_rec = REALMAX
        moderr_rec = REALMAX
    end if  ! End of IF (REDUCE_RHO). The procedure of reducing RHO ends.

    if (sum(xpt(:, kopt)**2) >= 1.0E2 * delta**2) then  ! 1.0E2 works better than 1.0E3 on 20230227.
        call shiftbase(kopt, xbase, xpt, zmat, bmat, pq, hq, idz)
    end if
end do  ! End of DO TR = 1, MAXTR. The iterative procedure ends.

```

Issues in the Fortran 77 implementation: an example

```fortran
C
C     If KNEW is zero initially, then pick the index of the interpolation
C       point to be deleted, by maximizing the absolute value of the
C       denominator of the updating formula times a weighting factor.
C
C
      IF (KNEW .EQ. 0) THEN
          DENMAX=ZERO
          DO 100 K=1,NPT
          HDIAG=ZERO
          DO 80 J=1,NPTM
          TEMP=ONE
          IF (J .LT. IDZ) TEMP=-ONE
   80     HDIAG=HDIAG+TEMP*ZMAT(K,J)**2
          DENABS=DABS(BETA*HDIAG+VLAG(K)**2)
          DISTSQ=ZERO
          DO 90 J=1,N
   90     DISTSQ=DISTSQ+(XPT(K,J)-XPT(KOPT,J))**2
          TEMP=DENABS*DISTSQ*DISTSQ
          IF (TEMP .GT. DENMAX) THEN
              DENMAX=TEMP
              KNEW=K
          END IF
  100     CONTINUE
      END IF
C
C     Apply the rotations that put zeros in the KNEW-th row of ZMAT.
C
      JL=1
      IF (NPTM .GE. 2) THEN
          DO 120 J=2,NPTM
          IF (J .EQ. IDZ) THEN
              JL=IDZ
          ELSE IF (ZMAT(KNEW,J) .NE. ZERO) THEN
```

The above code may crash, as KNEW may be used uninitialized.

Issues in the Fortran 77 implementation

- The Fortran 77 solvers may crash with memory violations (segfaults).
  Reason: Some indices are only initialized under conditions that can never be met because of NaN resulted from floating point exceptions.
- The Fortran 77 solvers may get stuck in infinite loops.
  Reason: Some loops are only terminated under conditions that can never be met because of NaN resulted from floating point exceptions.

N.B.:

- The problems are due to floating point exceptions in the Fortran 77 code rather than flaws in the algorithms.
- The problems affect all implementations or wrappers of these solvers based on the Fortran 77 code, including SciPy (COBYLA), NLopt, ...

How to ensure PRIMA does not have similar issues?

Strategy 1. Programming by contract

```
! Preconditions
if (DEBUGGING) then
    call assert(n >= 1 .and. npt >= n + 2, 'N >= 1, NPT >= N + 2', srname)
    call assert(delta > 0, 'DELTA > 0', srname)
    call assert(size(gopt_in) == n, 'SIZE(GOPT) = N', srname)
    call assert(size(hq_in, 1) == n .and. issymmetric(hq_in), 'HQ is an NxN symmetric matrix', srname)
    call assert(size(pq_in) == npt, 'SIZE(PQ) = NPT', srname)
    call assert(all(is_finite(xpt)), 'XPT is finite', srname)
    call assert(size(s) == n, 'SIZE(S) == N', srname)
end if
```

```
! Postconditions
if (DEBUGGING) then
    call assert(size(s) == n .and. all(is_finite(s)), 'SIZE(S) == N, S is finite', srname)
    ! Due to rounding, it may happen that ||S|| > DELTA, but ||S|| > 2*DELTA is highly improbable.
    call assert(norm(s) <= TWO * delta, '||S|| <= 2*DELTA', srname)
    call assert(crvmin >= 0, 'CRVMIN >= 0', srname)
end if
```

- The preconditions and postconditions are checked only in the debug mode. In the code that users receive, they are disabled by default.
- In the debug mode, if some subroutine receives strange inputs or produces strange outputs, the program will raise an error so that the developer (i.e., Zaikun Zhang) can check the issue and fix it.

How to ensure PRIMA does not have similar issues?

Strategy 2. TOUGH (Tolerance Of Untamed and Genuine Hazards) tests

```
function f = noisy(f, x, noise_level)
if nargin < 3
    noise_level = 2e-1;
end
r = cos(1.0D6 * sin(1.0D6 * (abs(f) + 1.0D0) * cos(1.0D6 * sum(abs(x)))));
f = f*(1+noise_level*r);
if (r > 0.9)
    error('Function evaluation fails!');
elseif (r > 0.75)
    f = inf;
elseif (r > 0.5)
    f = NaN;
elseif (r < - 0.999)
    f = -1e30;
end
return
```

- In TOUGH tests, objective functions are corrupted as above with `NaN`, `Inf`, evaluated failures, ..., and then fed to the solvers.
- PRIMA works properly even if the objective functions are corrupted in this severe way. (What about your solvers?)

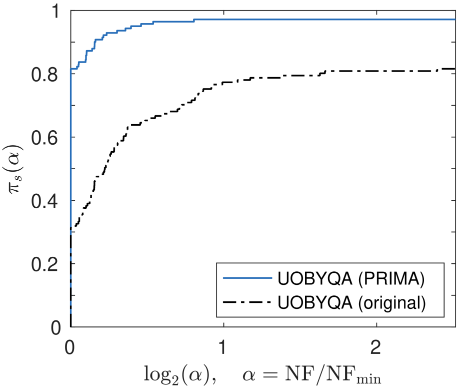
How to ensure PRIMA does not have similar issues?

Strategy 3. Automated and randomized tests using GitHub Actions

- Every day, extensive TOUGH tests and other tests are conducted automatically on randomized variants of CUTEst problems.
- The longer time passes, the more reliable PRIMA is, automatically.
- As of June 2023, $>$ 42,000 workflows have been successfully run.
- Each workflow consists of $\sim$ 5 (sometimes more than 150) randomized tests, each test taking from tens of minutes to several hours.
- In other words, PRIMA has been verified by more than 200,000 hours (or more than 20 years) of randomized tests.

Code must be battle-tested before it becomes software.

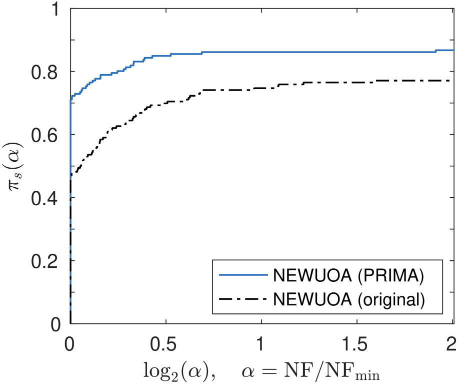
The performance of PRIMA



UOBYQA

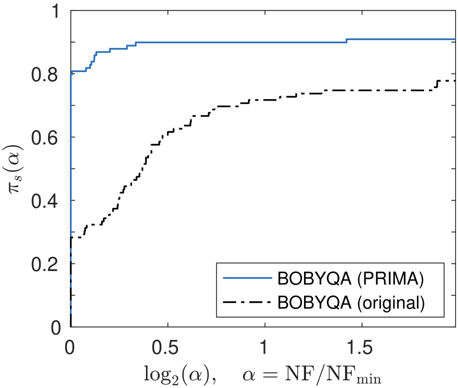
(unconstrained problems, at most 100 variables)

The performance of PRIMA



NEWUOA

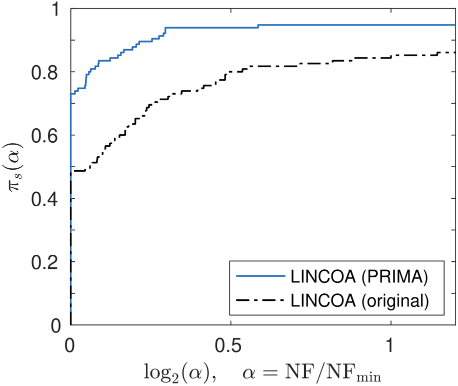
(unconstrained problems, at most 200 variables)



BOBYQA

(bound-constrained problems, at most 200 variables)

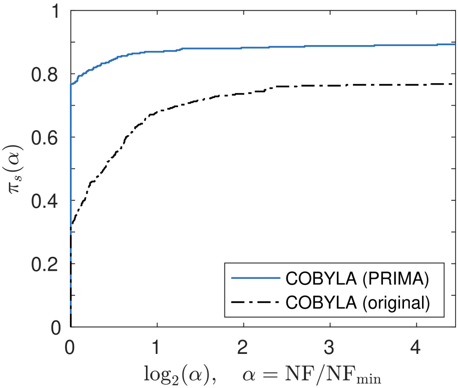
The performance of PRIMA



LINCOA

(linearly constrained problems, at most 200 variables, 20,000 constraints)

The performance of PRIMA



COBYLA

(nonlinearly constrained problems, at most 100 variables, 10,000 constraints)

How to ensure the improvements are not by luck?

Take COBYLA as an example.

The PRIMA implementation of COBYLA is tested on 359 nonlinearly constrained CUTEst problems with at most 100 variables and 10,000 constraints. Seven tests are made.

1. A plain test
2. A test that permutes the variables randomly
3. A test that perturbs the starting point randomly
4. A test based on single-precision objective & constraint values
5. A test using only 5 significant digits of the objective & constraints
6. A test contaminating the objective & constraints by deterministic noise
7. A test contaminating the objective & constraints by random noise

How to ensure the improvements are not by luck?

168 performance profiles of the new and old implementations of COBYLA

A "fun" fact ...

- Working on PRIMA, I have spotted a dozen of bugs in reputable Fortran compilers and two bugs in MATLAB.
- Each of them represents days of bitter debugging.
- From an unusual angle, they reflect how intensive the coding is.
- The bitterness behind this fun fact is exactly why I work on PRIMA:
  - I hope all the frustrations that I have experienced will not happen to any user of Powell's methods anymore.
  - I hope I am the last one in the world to decode a maze of 244 GOTOs in 7939 lines of Fortran 77 code — I did this for three years and I do not want anyone else to do it again.

But it is not quite rewarding in terms of career and life ...

- You may write 3 good papers in 1 year, but not 1 good package in 3 years, especially if you start with a nontrivial Fortran 77 codebase.
- Internet: "Writing software is a low-status academic activity."
- Internet: "A general problem is that ... professors are usually rewarded for publications, not their software."
- Comments on my grant proposal: The PI's expertise seems in software development, but he may not be a good mathematician.
- As a "not-so-good mathematician", I much prefer spending my time on proofs, which are a lot easier and much more enjoyable for me.
- Sometimes we do things that are not enjoyable but have to be done.

- Who translated Euclid's Elements to modern languages?
- You probably do not know (and do not care).
But we cannot live in a world without such a translation.

Concluding remarks

- Implementation of model-based DFO solvers is intrinsically hard
- PRIMA provides the reference implementation of Powell's DFO solvers
- The modern Fortran version and a MATLAB interface is finished
- PRIMA will also be implemented in MATLAB, Python, Julia, R, C++
- PRIMA fixes issues in the original Fortran 77 code
- PRIMA is tested extensively to ensure its correctness & robustness
- PRIMA outperforms the original implementation of the solvers

libprima.net

Thank you!