Numerics in LP and MIP solvers

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Numerical trouble and inaccuracies

```
SCIP> display solution

objective value:                     147726.165057267
x2826                                               1   (obj:13.8132)
x2840                                               1   (obj:17.3592)
x2842                                 1.000000000318   (obj:17.2398)
x2845                                               1   (obj:12)
x2850                                               1   (obj:12.1173)
x2851                                 0.999999999301   (obj:14.4105)
x2852                                 0.999999999987   (obj:12)
x2854                                               1   (obj:14.9862)
x2857                                               1   (obj:18.7107)
x2861                                               1   (obj:15.7479)
```

Numerical trouble and inaccuracies

```
  9.7s|     1 |     0 |  3507 |     - |   154M |   0 |2712 |  13k|  13k|  68 |  8 |  18 |   0 | 9.625279e+04 | 3.723994e+05 | 286.90%| unknown
 10.5s|     1 |     0 |  3645 |     - |   157M |   0 |2712 |  13k|  13k|  93 |  9 |  18 |   0 | 9.625416e+04 | 3.723994e+05 | 286.89%| unknown
 11.0s|     1 |     0 |  3718 |     - |   158M |   0 |2712 |  13k|  13k| 110 | 10 |  18 |   0 | 9.625435e+04 | 3.723994e+05 | 286.89%| unknown
 11.1s|     1 |     0 |  3782 |     - |   160M |   0 |2712 |  13k|  13k| 124 | 11 |  18 |   0 | 9.625474e+04 | 3.723994e+05 | 286.89%| unknown
 11.3s|     1 |     0 |  3893 |     - |   161M |   0 |2712 |  13k|  13k| 144 | 12 |  18 |   0 | 9.625534e+04 | 3.723994e+05 | 286.89%| unknown
 time | node  | left  |LP iter|LP it/n|mem/heur|mdpt |vars |cons |rows |cuts |sepa|confs|strbr|  dualbound   | primalbound  |  gap   | compl.
 24.3s|     1 |     2 | 35722 |     - |   163M |   0 |2712 |  13k|  13k| 144 | 12 |  44 |  19 | 9.626681e+04 | 3.723994e+05 | 286.84%| unknown
(node 5) numerical troubles in LP 104 -- unresolved
L 129s|    76 |    73 |127950 |1663.7 |    alns|  20 |2712 |  13k|  13k| 264 |  2 |  75 | 519 | 9.628491e+04 | 3.530913e+05 | 266.72%| unknown
  144s|   100 |    97 |148598 |1469.0 |   187M |  23 |2712 |  13k|  13k| 285 |  1 |  94 | 553 | 9.628491e+04 | 3.530913e+05 | 266.72%| unknown
```

Numerical trouble and inaccuracies

```
2800s| 93200 |   348 |  4749k|  49.7 |   253M |  55 | 289 |1925 |1764 | 207k|  0 |5691 |8539 | 3.027253e+03 | 3.336240e+03 |  10.21%|  98.40%

SCIP Status        : problem is solved [optimal solution found]
Solving Time (sec) : 2802.85
Solving Nodes      : 93263 (total of 95347 nodes in 2 runs)
Primal Bound       : +3.33623984845755e+03 (43 solutions)
Dual Bound         : +3.33623984845755e+03
Gap                : 0.00 %
[linear] <c13452>:  -0.002186551<x12>[C] (+38233.728) +<x47>[C] (+85.2158153) +1600000<x477>[B] (+0) +1600000<x622>[I] (-1.15885912e-11)
+1600000<x682>[I] (+0) >= 1.615819082;
                                         ;
violation: left hand side is violated by 1.85415070872441e-05
best solution is not feasible in original problem
```

1. Introduction

2. Floating-point arithmetic and MIP tolerances

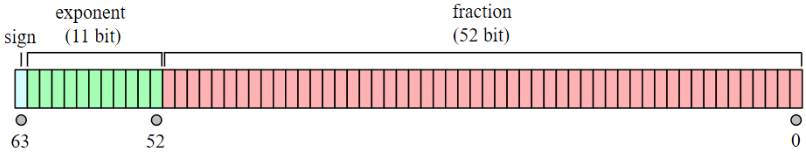
3. Some guidelines and tools

4. Iterative refinement for LP

5. Solving MIPs exactly

Floating-point arithmetic

Virtually all MIP solvers are built on double-precision floating-point arithmetic (IEEE754):



- Real numbers stored as $(-1)^{\text{sign}} \cdot 1.\text{fraction} \cdot 2^{\text{exponent}-1023}$
- enough to represent about 15 digits $\rightsquigarrow$ round-off errors afterwards, e.g.

$$\frac{1}{3} =_{fp} 0.333333333333333314829 6\ldots$$

$$3,000,000 \cdot \frac{1}{3} - 1,000,000 =_{fp} 0.00000000148296\ldots$$

$$3,000,000,000,000 \cdot \frac{1}{3} - 1,000,000,000,000 =_{fp} 0.00148296\ldots$$

Feasibility and optimality in floating-point solvers

MIP solvers use numerical tolerances, typically in the range 10^{-6} to 10^{-9}:

- Integrality tolerance ϵ_{int} : $\quad \alpha \in \mathbb{Z} \Leftrightarrow_{\mathit{tol}} \alpha \in \mathbb{Z} + [-\epsilon_{\mathit{int}}, \epsilon_{\mathit{int}}]$, e.g., $0.9999999 =_{\mathit{tol}} 1$.

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Absolute: $a^T x - b \leq \epsilon_{feas}$

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Relative: $$\frac{a^T x - b}{|b|} \leq \epsilon_{feas}$$

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Relative: $$\frac{a^T x - b}{|b|} \leq \epsilon_{feas}$$ (problematic for $|b| \approx 0$)

Mixed (SCIP): $$\frac{a^T x - b}{\max\{|b|, 1\}} \leq \epsilon_{feas}$$

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Mixed (SCIP):	$\dfrac{a^T x - b}{\max\{\lvert b \rvert, 1\}} \leq \epsilon_{feas}$	

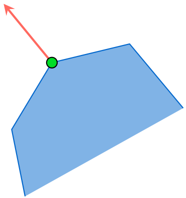
- LP tolerances for dual feasibility, barrier convergence, ...

Note: **not invariant under scaling**!

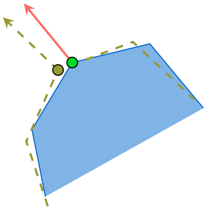
Feasibility and optimality in floating-point solvers

Hope:
Optimal solution with small residual errors is
close to an exact optimal solution without violations.

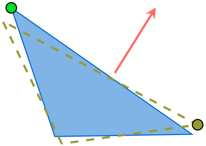
But really: exact solution to a **perturbed problem**



exact solution



good case



bad case

Sources of numerical issues: large big-M's

Example:

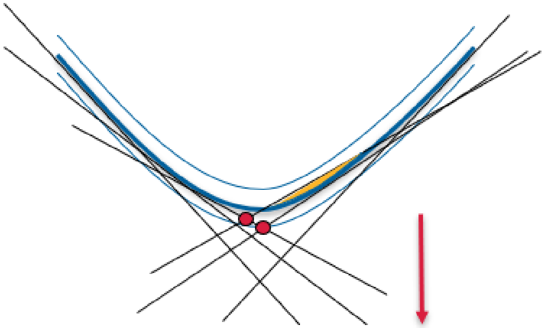
$$\begin{aligned} \min\ & x \\ \text{s.t. } & x \geq 1 \\ & x \leq 10^6 y \\ & y \in \{0,1\} \end{aligned} \qquad\qquad \begin{aligned} \min\ & x \\ \text{s.t. } & x \geq 1 \\ & 10^{-6} x \leq y \\ & y \in \{0,1\} \end{aligned}$$

Assuming an absolute tolerance of 10^{-6}, we have that:

- $x = 1, y = 0$ feasible in the scaled problem w.r.t. tolerances, but infeasible in the original
- $x = 1, y = 10^{-6}$ feasible in both, the scaled and original problem w.r.t. tolerances
- but when you fix $y = 0$ and reoptimize, the result will be infeasible
- $x = y = 1$ is exactly feasible

Sources of numerical issues: in MINLP solving

- Approximating convex functions by cutting planes can yield near-parallel rows in the LP and ill-conditioned basis matrices.
- Relaxations of nonconvex constraints over large domains can yield bad coefficients.
- ...



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3. **Some guidelines and tools**
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Some guidelines

- Good input, good output
  - Scale data to avoid extreme values: absolute and relative
    look at which units to use, e.g.
    ratio of largest to smallest coefficient $\leq 10^6$ in any row and column
  - Ensure that tolerances make sense relative to the input data.
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- Modelling and solving
  - Try different scaling parameters
  - Try to avoid large big-M's
  - If you don't have a reasonable *M*, use indicator or SOS constraints
  - If the objective is a hierarchical combination of multiple objective:
    try a sequential approach (akin to the ϵ-constraint method)

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  - If the objective is a hierarchical combination of multiple objective:
    try a sequential approach (akin to the ϵ-constraint method)
- Note: Poor scaling and imprecise input are **neither necessary nor sufficient** for numerical problems.

Tools: a posteriori

```
SCIP> checksol

check best solution
solution is feasible in original problem
Violation            :    absolute     relative
  bounds             : 3.18000e-10 3.18000e-10
  integrality        : 3.18000e-10           -
  LP rows            : 1.47428e-09 1.47428e-09
  constraints        : 1.47428e-09 1.47428e-09
```

Tools: a priori

```
Running HiGHS 1.7.2 (git hash: 8fce6250c): Copyright (c) 2024 HiGHS under MIT licence terms
Number of PL entries in BOUNDS section is 45
LP   mwe has 4203 rows; 194 cols; 23776 nonzeros
Coefficient ranges:
  Matrix [1e-09, 1e+07]
  Cost   [8e-02, 2e+00]
  Bound  [1e+03, 1e+06]
  RHS    [1e-13, 4e+11]
WARNING: Problem has excessively large bounds or RHS: consider scaling the bounds and RHS down
by at least 1e+2, or setting option user_bound_scale to -6 or less
```

Tools: check solver log during optimization

```
Warning: Model contains large matrix coefficient range
Consider reformulating model or setting
NumericFocus parameter to avoid numerical issues.
Warning: Markowitz tolerance tightened to 0.5
Warning: switch to quad precision
Numeric error
Numerical trouble encountered
Restart crossover...
Sub-optimal termination
Warning: ... variables dropped from basis
Warning: unscaled primal violation = ... and residual = ...
Warning: unscaled dual violation = ... and residual = ...
```

Tools: condition numbers

- Condition number κ of a matrix:
  bounds how error in the right-hand side can propagate to the solution vector

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  bounds how error in the right-hand side can propagate to the solution vector
- For the simplex method: large κ of basis matrices indicates larger errors in the LP solutions
- For LP-based branch and bound: can compute or sample a “MIP-κ” / “attention level” / …as a **weighted average of encountered LP-κ’s**

Numerical information – Xpress final report

glass4 with default scaling:

```
Numerical issues encountered:
   Dual failures      :   3410 out of    508042 (ratio: 0.0067)
   Singular bases     :     18 out of    372616 (ratio: 0.0000)
   Nodes kappa stable      :          0 (ratio: 0.0000)
   Nodes kappa suspicious  :          0 (ratio: 0.0000)
   Nodes kappa unstable    :        260 (ratio: 0.0008)
   Nodes kappa ill-posed   :     307910 (ratio: 0.9992)
   Largest kappa seen      : 5.166264e+22
   Kappa attention level   : 0.9994
```

glass4 with SCALING=227 [scale big-M rows]

```
Numerical issues encountered:
   Dual failures      :    683 out of    531681 (ratio: 0.0013)
   Singular bases     :      4 out of    401058 (ratio: 0.0000)
   Nodes kappa stable      :     240371 (ratio: 0.8744)
   Nodes kappa suspicious  :      34412 (ratio: 0.1252)
   Nodes kappa unstable    :        102 (ratio: 0.0004)
   Nodes kappa ill-posed   :          0 (ratio: 0.0000)
   Largest kappa seen      : 1.654603e+12
   Kappa attention level   : 0.0014
```

Gurobi's model analyzer

GUROBI
OPTIMIZATION

Gurobi Model Analyzer

Search

CONTENTS:

Installation

Ill Conditioning Explainer

Quick Start Guide

Ill Conditioning Explainer

- Quick Start Guide
  - Introduction
  - Running the Explainer
  - Interpreting the Output
  - Suggested Usage Quick Start
- Advanced Usage Guide
  - Introduction
  - Interpreting the Explainer Output
  - Additional Function Arguments
- API Reference
  - `gurobi_modelanalyzer.kappa_explain()`

Xpress's solution refiner

Goal: reduce or remove primal, dual and integrality violations in incumbents and final solution by some of

- performing extra simplex iterations
- recomputing in quad precision
- pushing fractional integer variables out of the basis when possible
- performing additional branches to force integer variables to integer values
- fixing integer variables and solve remaining LP

```
    Node      BestSoln     BestBound    Sols Active  Depth     Gap     GInf   Time
*    197   15183.85668  15227.15725      8      1     19    0.28%       0      3
     200   15183.85668  15220.67819      8      1      8    0.24%       5      3
 *** Search completed ***     Time:      4 Nodes:        253
Number of integer feasible solutions found is 8
Best integer solution found is  15183.85668
Best bound is  15183.85668
Refining MIP solution (1.116e-06 fractionality 3.617e-05 abs infeasiblity)
P    253   15183.86782  15183.85668      9      0     10    0.00%       0      4
Refined MIP solution (0.0 fractionality 9.890e-07 abs infeasiblity)
```

MIP-DD: A Delta-Debugger for MIP

Goal: try to reproduce unwanted behavior in a MIP solver, e.g., a numerical issue, on a significantly smaller and easier to analyze MIP

- inspired by **delta debugging** heavily used in the SAT and SMT community (Zeller 1999, Brummayer and Biere 2009, Niemetz and Biere 2013, Kaufmann and Biere 2022, Paxian and Biere 2023)
- very successful in increasing the number of bug fixes in the last SCIP releases
- open-source package MIP-DD available at `github.com/scipopt/mip-dd`
- for details see Hoen, Kampp, G. 2024: "MIP-DD: A Delta Debugger for Mixed Integer Programming Solvers", `arxiv.org/abs/2405.19770v1`

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Recall

Basic solution: primal-dual

- W.l.o.g. let $rank(A) = m < n$ and consider the computational form

$$\min\{c^T x \mid Ax = b, x \geq 0\} = \max\{y^T b \mid y^T A \leq c, y \text{ free}\}$$

- For every vertex there is a non-singular $m \times m$ sub-matrix B of A

$$A = \begin{bmatrix} B & N \end{bmatrix}$$

- and the corresponding basic solution is given by

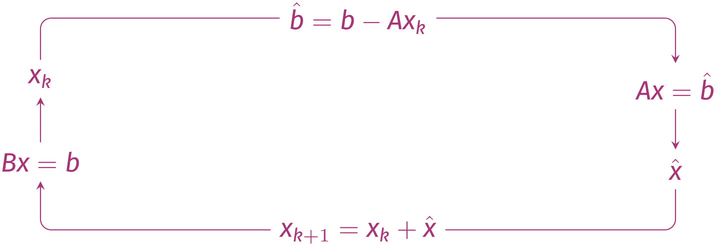
$$x_B = B^{-1}b, \qquad x_N = 0, \qquad y^T = c_B^T B^{-1}$$

- In practice: do not compute inverse, but solve linear systems $Bx_B = b$ and $B^T y = c_B$ by factorization $B = LU$
- Floating-point arithmetic results in residual errors $\hat{b} = b - Bx_B \neq 0$ and $\hat{c} = c_B - B^T y \neq 0$.

Iterative refinement for linear systems

(Wilkinson 1963, Ursic and Patarra 1983, Wan 2006, Pan 2011, Saunders et al. 2011)

- Drop subscript $x_B \rightsquigarrow x$ and suppose we want to solve $Bx = b$
- Idea: compute corrector solution $\hat{x}$ by using residual error as the right-hand side



Hybrid precision method: fast floating-point arithmetic (for linear system solve)
+ slower extended-precision or rational arithmetic (for residual computation and correction)

Iterative refinement for linear programs

(G., Steffy, Wolter 2012, 2016, 2020)

$$
\begin{aligned}
P : \mathbf{min} \quad & c^T x \\
\mathbf{s.\,t.} \quad & Ax = b \\
& x \geq \ell
\end{aligned}
$$

Iterative refinement for linear programs

(G., Steffy, Wolter 2012, 2016, 2020)

$$x_k, y_k$$

$$\uparrow$$

$$\begin{aligned} P : \min \quad & c^T x \\ \text{s.t.} \quad & Ax = b \\ & x \geq \ell \end{aligned}$$

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$$\hat{b} = b - Ax_k, \hat{\ell} = \ell - x_k, \hat{c} = c - A^T y_k$$

$$x_k, y_k$$

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$$x_k, y_k$$

$$P: \min\ c^T x \quad \text{s.t.}\quad Ax = b,\quad x \geq \ell$$

$$\hat{P}: \min\ \Delta_k \hat{c}^T x \quad \text{s.t.}\quad Ax = \Delta_k \hat{b},\quad x \geq \Delta_k \hat{\ell}$$

Iterative refinement for linear programs

(G., Steffy, Wolter 2012, 2016, 2020)

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$$\hat{x}, \hat{y}$$

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(G., Steffy, Wolter 2012, 2016, 2020)

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$$\uparrow$$

$$x_k, y_k$$

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$$\hat{P} : \min \; \Delta_k \hat{c}^T x \quad \text{s.t.} \quad Ax = \Delta_k \hat{b}, \quad x \geq \Delta_k \hat{\ell}$$

$$\downarrow$$

$$\hat{x}, \hat{y}$$

$$x_{k+1} = x_k + \frac{1}{\Delta_k}\hat{x}, \; y_{k+1} = y_k + \frac{1}{\Delta_k}\hat{y}$$

Iterative refinement for linear programs

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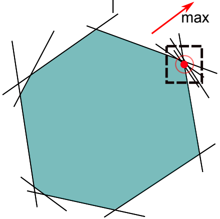
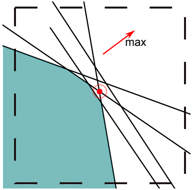


$$\Delta_k \to \infty$$



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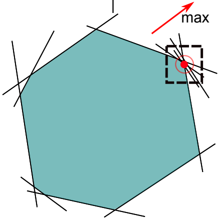
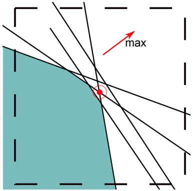


$$\Delta_k \to \infty$$



$$x_{k+1} = x_k + \frac{1}{\Delta_k}\hat{x},\ y_{k+1} = y_k + \frac{1}{\Delta_k}\hat{y}$$

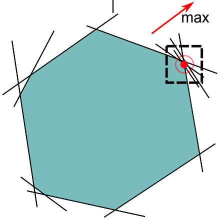
Hybrid precision method: double precision (for simplex)

+ rational arithmetic (for error computation, correction, rounding, LU)

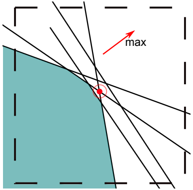
Boosted Iterative refinement for linear programs

(Applegate et al. 2007 + G., Steffy, Wolter 2012, 2016, 2020+ $\to$ G., Nicolas-Thouvenin, Eifler 2024)

$$\hat{b} = b - Ax_k, \hat{\ell} = \ell - x_k, \hat{c} = c - A^T y_k$$



$$\Delta_k \to \infty$$



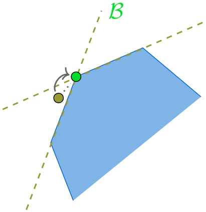
$$x_{k+1} = x_k + \frac{1}{\Delta_k}\hat{x}, y_{k+1} = y_k + \frac{1}{\Delta_k}\hat{y}$$

Hybrid precision method: double + extended precision (for simplex)
+ rational arithmetic (for error computation, correction, rounding, LU)

From accurate to exact

Method 1: Basis Verification

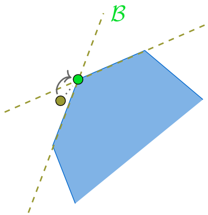
- compute exact basic solution via rat. LU factorization
- check primal and dual feasibility
- keep refining until optimal



From accurate to exact

Method 1: Basis Verification

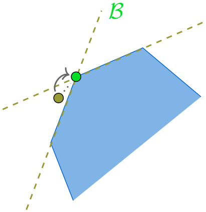
- compute exact basic solution via rat. LU factorization
- check primal and dual feasibility
- keep refining until optimal



Method 2: Output-Sensitive Rational Reconstruction

- round approximate solution by continued fractions approximation
- check primal and dual feasibility and complementary slackness
- increase denominator bound as residual errors decrease

From accurate to exact



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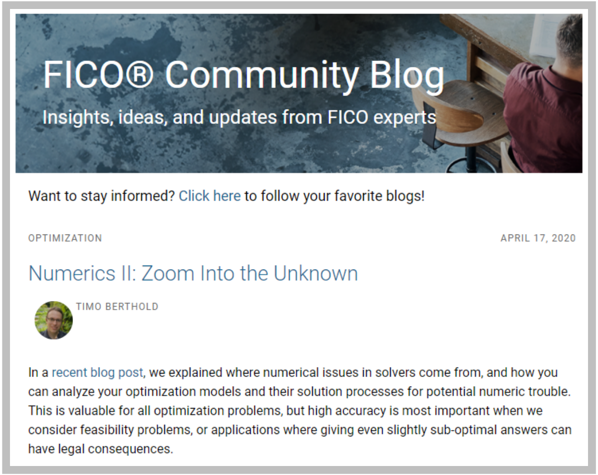
Can prove **oracle-polynomial running time** under some assumptions on the fp solver:
Exact solution reached after a polynomial number of refinements

- Method 1: $O((m^2\langle A\rangle + \langle b, c, \ell\rangle + n^2))$
- Method 2: $O(\max\{\log D, m^2\langle A\rangle\})$

Implemented in the open-source solver SoPlex: `github.com/scipopt/soplex`

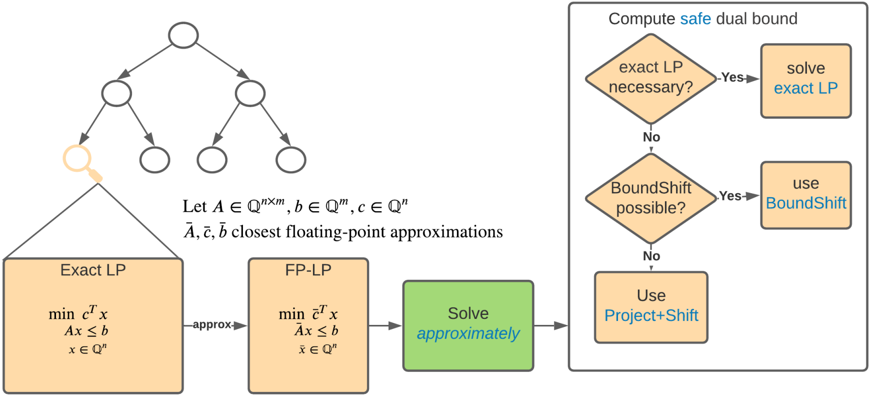
LP iterative refinement in industry

- Iterative refinement for solving linear systems in LP solvers is a standard technique to deal with ill-conditioned basis matrices,
- but also LP iterative refinement has been implemented with quad precision instead of rational arithmetic:
- see `community.fico.com/s/blog-post/a5Q2E000000cDPaUAM/fico2199`



1. Introduction
2. Floating-point arithmetic and MIP tolerances
3. Some guidelines and tools
4. Iterative refinement for LP
5. **Solving MIPs exactly**

From exact LP to exact MIP

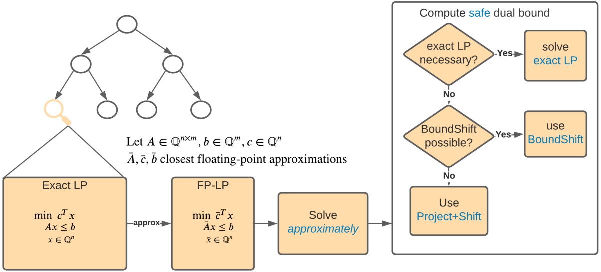


Hybrid-precision branch and bound (Cook, Koch, Steffy, Wolter 2013).

Uses floating-point + directed rounding + rational arithmetic.

Exact SCIP: Hybrid-precision branch-and-bound plus ...

- primal repair heuristics
  (Eifler, G. 2022)
- rational presolving through PaPILO
  (G. Gottwald, Hoen 2023)
- propagation and dual proof analysis (Borst, Eifler, G. 2024)
- MIR cuts (Eifler, G. 2024)
- certificates (Cheung, G., Steffy 2017)



Available at `github.com/scipopt/scip/tree/exact-rational`.