Computer Algebra and the Formalisation of New Mathematics

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Formalisation Seminar, DPMMS, 21 November 2024

Computer Algebra and Formal Proof

A and B are both nice: why not A&B?

Three decades of trying to combine CA and ATP

"Computer algebra is unsound"

"CA tools can't reason logically"

Approaches: certificates, tightly constrained oracles, reflection

Often missing: a compelling *application*

Computer algebra techniques within Isabelle/HOL

- Differentiation and integration
- Automatic asymptotic / limit proofs
- Arbitrary precision calculations by interval arithmetic
- Real & complex root-finding, counting winding numbers, and other specialised proof methods

Symbolic differentiation

Let's differentiate $e^{-t}\cos(2\pi t)$ by proof alone

lemma "∃f'. ((\u03c0 x. exp(-x)*cos(2*pi*x)) has_real_derivative f' t) (at t) \u03c0 P(f' t)" for t
apply (rule exI conjI derivative_eq_intros)+

(just a partial step to reveal what's going on:)

```
goal (6 subgoals):
1. 1 = ?f'15
2. - ?f'15 = ?Db11
3. exp (- t) * ?Db11 = ?Da6
4. ((λx. cos (2 * pi * x)) has_real_derivative ?Db6) (at t)
5. ?Da6 * cos (2 * pi * t) + ?Db6 * exp (- t) = ?f' t
6. P (?f' t)
```

To do it properly, we must supply a *tactic* to prove the equality subgoals

lemma "∃f'. ((\u03c0 x. exp(-x)*cos(2*pi*x)) has_real_derivative f' t) (at t) \u03c0 P(f' t)" for t
_ apply (rule exI conjI derivative_eq_intros | force)+

The result is (sometimes) even simplified!

goal (1 subgoal):
 1. P (- (exp (- t) * cos (2 * pi * t)) sin (2 * pi * t) * (2 * pi) * exp (- t))

 $-e^{-t}\cos(2\pi t) - \sin(2\pi t) \cdot 2\pi e^{-t}$

Symbolic integration (cheating with Maple)

$$x^{2} \cdot \cos(4 \cdot x) \xrightarrow{\text{integrate w.r.t. } x} \frac{x^{2} \sin(4x)}{4} - \frac{\sin(4x)}{32} + \frac{x \cos(4x)}{8}$$

Just ask Isabelle to *check* Maple by taking the derivative:

This time, the output is ugly

```
goal (1 subgoal):
1. ((real 2 * (1 * x ^ (2 - Suc 0)) * sin (4 * x) +
        cos (4 * x) * (0 * x + 1 * 4) * x<sup>2</sup>) *
        4 -
        x<sup>2</sup> * sin (4 * x) * 0) /
        (4 * 4) -
        (cos (4 * x) * (0 * x + 1 * 4) * 32 - sin (4 * x) * 0) /
        (32 * 32) +
        ((1 * cos (4 * x) + - sin (4 * x) * (0 * x + 1 * 4) * x) * 8 -
        x * cos (4 * x) * 0) /
        (8 * 8) =
        x<sup>2</sup> * cos (4 * x)
```

... but easy to fix:

apply (simp add: field_simps)
done

We can even evaluate *definite integrals* via the fundamental theorem of calculus

Eberl's real asymptotics package

- Proves claims about limits, properties holding in the limit, claims involving Landau symbols
- ... by computing *multiseries expansions* for a variety of real-valued functions (cf Richardson et al., 1996).
- All by inference alone!

$$\lim_{x \to 0} \frac{1 - \frac{1}{2}x^2 - \cos\left(\frac{x}{1 - x^2}\right)}{x^4} = \frac{23}{24}$$

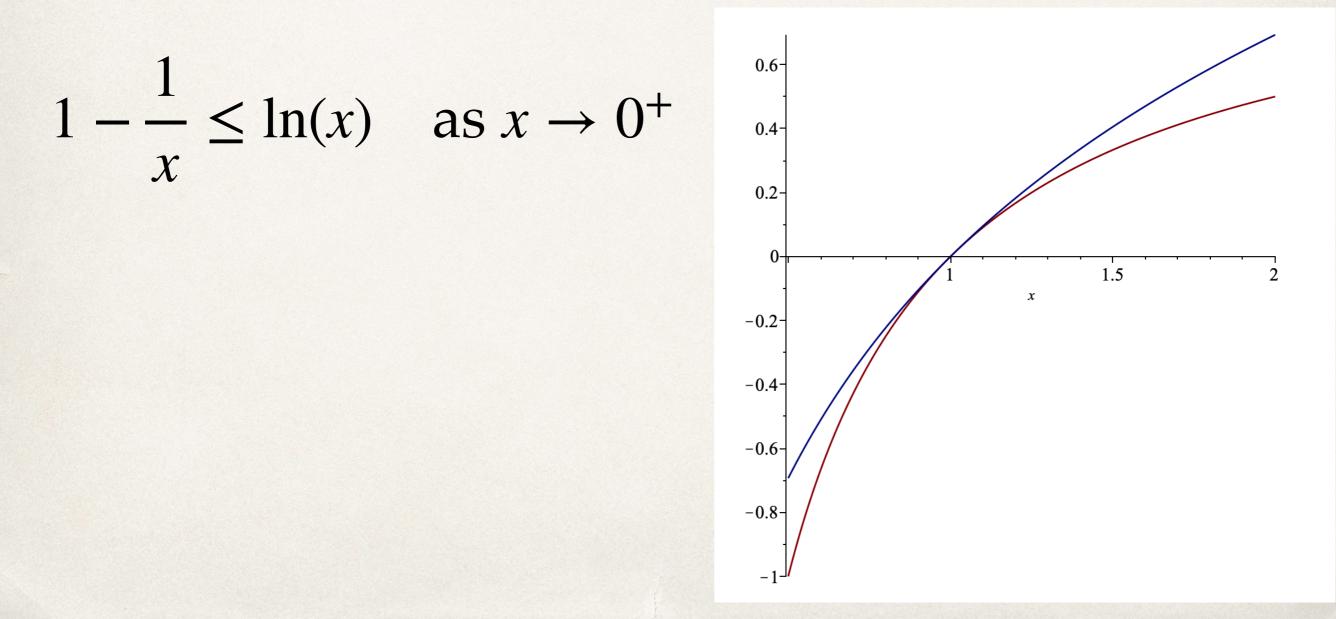
lemma "(λx::real. (1 - 1/2 * x² - cos (x / (1 - x²))) / x⁴) −0→ 23/24"
by real_asymp

$$n^k = o(c^n)$$

lemma "c > 1 \implies (λ n. real n ^ k) \in o(λ n. c^n)" by real_asymp

Can even do one-sided limits

lemma "eventually (λx ::real. 1 - 1/x \leq ln(x)) (at_right 0)" **by** real_asymp



Exact numeric calculations

Simple inequalities:

lemma "| sin 100 + 0.50636564110975879 | < (inverse 10 ^ 17 :: real)"
by (approximation 70)</pre>

Inequalities over a range of inputs:

lemma "0.5 \leq x \land x \leq 4.5 \implies ; arctan x - 0.91 ; < 0.455"
by (approximation 10)</pre>

Going beyond interval arithmetic:

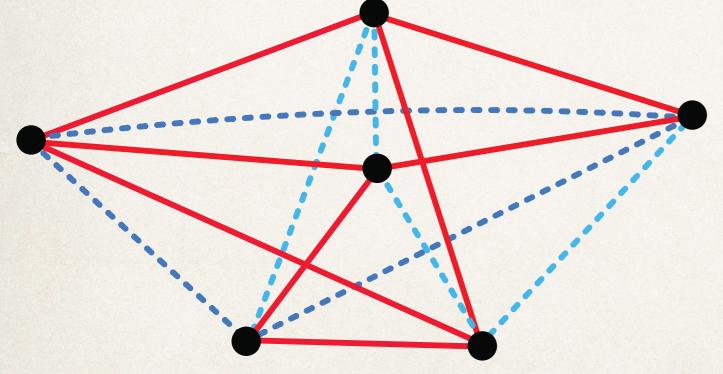
```
lemma "x \in { 0 .. 1 :: real } \longrightarrow x<sup>2</sup> \leq x"
by (approximation 30 splitting: x=1 taylor: x = 3)
```

But is there an application?

Ramsey's Theorem

"Party Problem" version (2-sets)

For all *m* and *n* there exists a number R(m, n) such that every graph with at least R(m, n) vertices contains a *clique* of size *m* or an *anti-clique* of size *n*



Or: a complete graph with edges coloured red/blue contains a *red clique* of size *m* or a *blue clique* of size *n*

R(3,3) = 6

Other forms (for *r*-sets, $r \neq 2$)

r = 1: Ramsey's theorem is just the *pigeonhole principle*

r > 2: hypergraph form, with unimaginably large *Ramsey numbers*

The r = 2 case can also be generalised with *transfinite ordinals or cardinals*

Ramsey numbers

$$R(3,3) = 6$$
 $R(4,4) = 18$

Erdős (with Szekeres for the upper bound) proved

$$\sqrt{2}^k \le R(k,k) \le \binom{2k-2}{k-1} < 4^k$$

A new result replaces 4 by $4 - \epsilon$, an exponential improvement

 $43 \le R(5,5) \le 46$

"Algorithm" to prove the 4^k bound

A

x \bullet

At start: put all vertices in X; set $A = B = \{\}$ $X \to N_R(x) \cap X \quad A \to A \cup \{x\}$ if x has more red neighbours than blue in X $X \to N_B(x) \cap X \quad B \to B \cup \{x\}$ otherwise

Builds a red clique in *A*, a blue clique in *B*

- At each step, choose the vertex x arbitrarily
 - ✤ … the set *X* loses up to half its vertices
 - * ... there are only red edges to A, blue edges to B
- ★ If |X| ≥ 2^{k+ℓ} then iteration finally yields a clique:
 either |A| ≥ k or |B| ≥ ℓ
- * In the "diagonal" case $k = \ell$, the upper bound is 4^k

Could a more sophisticated algorithm do better?

A New Paper on Ramsey's Theorem

AN EXPONENTIAL IMPROVEMENT FOR DIAGONAL RAMSEY

MARCELO CAMPOS, SIMON GRIFFITHS, ROBERT MORRIS, AND JULIAN SAHASRABUDHE

ABSTRACT. The Ramsey number R(k) is the minimum $n \in \mathbb{N}$ such that every red-blue colouring of the edges of the complete graph K_n on n vertices contains a monochromatic copy of K_k . We prove that

$$R(k) \leqslant (4-\varepsilon)^k$$

for some constant $\varepsilon > 0$. This is the first exponential improvement over the upper bound of Erdős and Szekeres, proved in 1935.

First formalised, in Lean, by Bhavik Mehta: before the referees had completed their reviews!

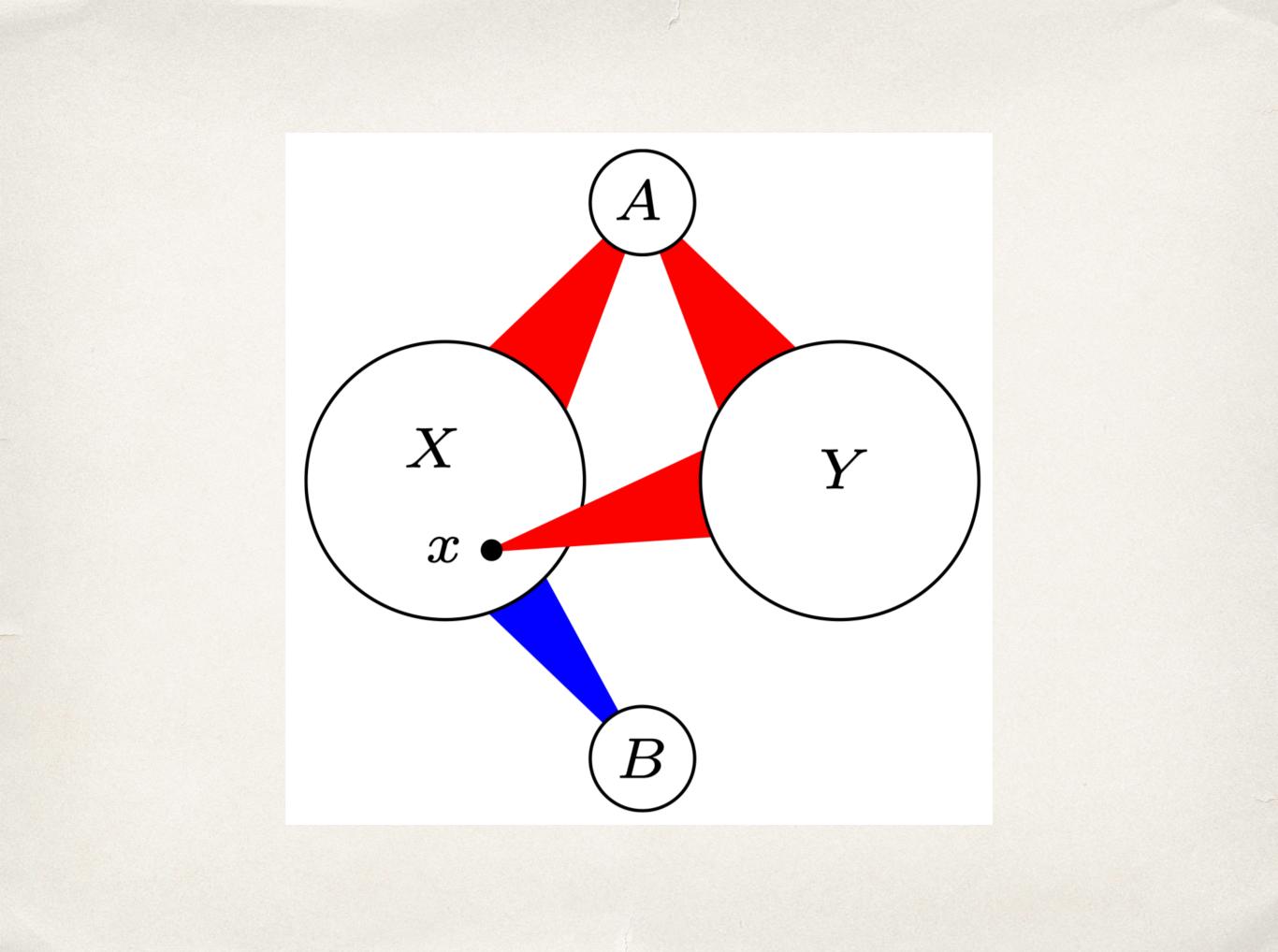
What's the mathematics like?

- A more complicated "book algorithm"
- A string of technical lemmas describing its behaviour
 - Numerous estimates with finite sums / products
 - Numeric parameters; high-precision calculations
 - Lots and lots of limit arguments

And it's 57 pages

The variables and their constraints

- * Integers $\ell \leq k$ and a complete *n*-graph
- Edge colouring with no red k-clique, no blue l-clique
- Sets of vertices X, Y, A, B, the latter two initially empty
- All edges between A and A, X, Y are red
- ✤ All edges between *B* and *B*, *X* are blue



Some mathematical preliminaries

Standard definitions for undirected graphs

As X and Y evolve, need to maintain a sufficient red density

$$p = \frac{e_R(X, Y)}{|X||Y|}$$

Algorithm tries to build a large red clique in A

The main execution steps

- Degree regularisation: remove from X all vertices with "few" red neighbours in Y
- *Big blue step*: If there exist *R*(*k*, [*t*^{2/3}]) vertices in *X* with "lots" of blue neighbours in *X*, move a block of them into *B* while leaving just their blue neighbours in *X*
- *Red* and *density-boost* steps: an element of X with "few" blue neighbours in X is moved into A or into B, according to the red density of the resulting X and Y

A red or density-boost step

 $X \to N_R(x) \cap X \qquad Y \to N_R(x) \cap Y \qquad A \to A \cup \{x\}$

versus

$X \to N_B(x) \cap X \qquad Y \to N_R(x) \cap Y \qquad B \to B \cup \{x\}$

resembles the basic algorithm, except that *x* is carefully selected

A Glimpse at the Proofs

Defining the "book algorithm"

```
definition next_state :: "[real,nat,nat,'a config] ⇒ 'a config" where
  "next_state ≡ λμ l k (X,Y,A,B).
    if many_bluish μ l k X
    then let (S,T) = choose_blue_book μ (X,Y,A,B) in (T, Y, A, B∪S)
    else let x = choose_central_vx μ (X,Y,A,B) in
        if reddish k X Y (red_density X Y) x
        then (Neighbours Red x ∩ X, Neighbours Red x ∩ Y, insert x A, B)
        else (Neighbours Blue x ∩ X, Neighbours Red x ∩ Y, A, insert x B)"

primrec stepper :: "[real,nat,nat,nat] ⇒ 'a config" where
    "stepper μ l k 0 = (X0,Y0,{},{})"
    "stepper μ l k (Suc n) =
        (let (X,Y,A,B) = stepper μ l k n in
```

```
if termination_condition l k X Y then (X,Y,A,B)
else if even n then degree reg k (X,Y,A,B) else next state \mu l k (X,Y,A,B))"
```

Many routine properties easily proved

A proof in more detail: Lemma 4.1

Lemma 4.1. Set $b = \ell^{1/4}$. If there are $R(k, \ell^{2/3})$ vertices $x \in X$ such that $|N_B(x) \cap X| \ge \mu |X|$,

then X contains either a red K_k , or a blue book (S,T) with $|S| \ge b$ and $|T| \ge \mu^{|S|} |X|/2$.

(9)

Four weeks, 354 lines and several buckets of sweat later...

lemma Blue_4_1:
 assumes "X⊆V" and manyb: "many_bluish X" and big: "Big_Blue_4_1 μ l"
 shows "∃S T. good_blue_book X (S,T) ∧ card S ≥ l powr (1/4)"

[The claim holds for **sufficiently large** *l* and *k*]

What did I do in those three weeks?

Proved the Erdős lower bound for Ramsey numbers, $2^{k/2} \le R(k,k)$

> Got to grips with neighbours, edge densities, convexity

figured out that most claims only **hold in the limit**

Formalised a second probabilistic proof

First half of the proof

Proof of Lemma 4.1. Let $W \subset X$ be the set of vertices with blue degree at least $\mu|X|$, set $m = \ell^{2/3}$, and note that $|W| \ge R(k, m)$, so W contains either a red K_k or a blue K_m . In the former case we are done, so assume that $U \subset W$ is the vertex set of a blue K_m . Let σ be the density of blue edges between U and $X \setminus U$, and observe that

$$\sigma = \frac{e_B(U, X \setminus U)}{|U| \cdot |X \setminus U|} \ge \frac{\mu |X| - |U|}{|X| - |U|} \ge \mu - \frac{1}{k}$$
(10)

since |U| = m and $|X| \ge R(k, m)$, and each vertex of U has at least $\mu|X|$ blue neighbours in X. Since $\mu > 0$ is constant, $b = \ell^{1/4}$ and $m = \ell^{2/3}$, it follows that $b \le \sigma m/2$.

> Bhavik changed this to 2

Inequalities frequently hold only in the limit

```
have "\mu * (card X - card U) \leq card (Blue \cap all edges betw un {u} (X-U)) + (1-\mu) * m"
  if "u \in U" for u
proof -
  have NBU: "Neighbours Blue u \cap U = U - \{u\}"
    using <clique U Blue> Red Blue all singleton not edge that
    by (force simp: Neighbours def clique def)
  then have NBX split: "(Neighbours Blue u \cap X) = (Neighbours Blue u \cap (X-U)) \cup (U - \{u\})"
    using \langle U \subset X \rangle by blast
  moreover have "Neighbours Blue u \cap (X-U) \cap (U - \{u\}) = \{\}"
    by blast
  ultimately have "card(Neighbours Blue u \cap X) = card(Neighbours Blue u \cap (X-U)) + (m - Suc 0)"
    by (simp add: card_Un_disjoint finite Neighbours <finite U> <card U = m> that)
  then have "\mu * (card X) \leq real (card (Neighbours Blue u \cap (X-U))) + real (m - Suc 0)"
    using W def \langle U \subseteq W \rangle bluish def that by force
  then have "\mu * (card X - card U)
          \leq card (Neighbours Blue u \cap (X-U)) + real (m - Suc 0) - \mu *card U"
    by (smt (verit) cardU less X nless le of nat diff right diff distrib')
  then have *: "\mu * (card X - card U) \leq real (card (Neighbours Blue u \cap (X-U))) + (1-\mu)*m"
    using assms by (simp add: <card U = m> left diff distrib)
  have "inj on (\lambda x. {u,x}) (Neighbours Blue u \cap X)"
    by (simp add: doubleton eq iff inj on def)
  moreover have "(\lambda x. {u,x}) ` (Neighbours Blue u \cap (X-U)) \subseteq Blue \cap all_edges_betw_un {u} (X-U)"
    using Blue E by (auto simp: Neighbours def all edges betw un def)
  ultimately have "card (Neighbours Blue u \cap (X-U)) \leq card (Blue \cap all edges betw un {u} (X-U))"
    by (metis NBX split Blue eq card image card mono complete fin edges finite Diff finite Int inj
  with * show ?thesis
    by auto
qed
```

Second half of the proof

Let $S \subset U$ be a uniformly-chosen random subset of size b, and let $Z = |N_B(S) \cap (X \setminus U)|$ be the number of common blue neighbours of S in $X \setminus U$. By convexity, we have

$$\mathbb{E}[Z] = \binom{m}{b}^{-1} \sum_{v \in X \setminus U} \binom{|N_B(v) \cap U|}{b} \ge \binom{m}{b}^{-1} \binom{\sigma m}{b} \cdot |X \setminus U|.$$
probabilistic argument

Now, by Fact 4.2, and recalling (10), and that $b = \ell^{1/4}$ and $m = \ell^{2/3}$, it follows that

$$\mathbb{E}[Z] \ge \sigma^b \exp\left(-\frac{b^2}{\sigma m}\right) \cdot |X \setminus U| \ge \frac{\mu^b}{2} \cdot |X|, \qquad (11)$$

and hence there exists a blue clique $S \subset U$ of size b with at least this many common blue neighbours in $X \setminus U$, as required.

Probabilistic proofs – commonplace in combinatorics – were introduced by Erdős

```
define \Omega where "\Omega \equiv nsets U b" — (Choose a random subset of size @{term b})
have card \Omega: "card \Omega = m choose b"
  by (simp add: \Omega def <card U = m>)
then have fin\Omega: "finite \Omega" and "\Omega \neq \{\}" and "card \Omega > 0"
  using \langle b \leq m \rangle not less by fastforce+
define M where "M \equiv uniform count measure \Omega"
interpret P: prob space M
  using M_def (b \leq m) card\Omega fin\Omega prob space uniform count measure by force
have measure_eq: "measure M C = (if C \subseteq \Omega then card C / card \Omega else 0)" for C
  by (simp add: M def fin\Omega measure uniform count measure if)
define Int NB where "Int NB \equiv \lambda S. \bigcap v \in S. Neighbours Blue v \cap (X-U)"
have sum card NB: "(\sum A \in \Omega. card (\bigcap(Neighbours Blue ` A) \cap Y))
                    = (\sum v \in Y. card (Neighbours Blue v \cap U) choose b)"
  if "finite Y" "Y < X-U" for Y</pre>
  using that
proof (induction Y)
  case (insert y Y)
  have *: "\Omega \cap \{A, \forall x \in A, y \in Neighbours Blue x\} = nsets (Neighbours Blue y \cap U) b"
    "\Omega \cap - {A. \forall x \in A. y \in Neighbours Blue x} = \Omega - nsets (Neighbours Blue y \cap U) b"
    "[Neighbours Blue y \cap U] pb_{\aleph} \subseteq \Omega"
    using insert.prems by (auto simp: \Omega def nsets def in Neighbours iff insert commute)
  then show ?case
    using insert fin\Omega
    by (simp add: Int insert right sum Suc sum. If cases if distrib [of card]
         sum.subset diff flip: insert.IH)
qed auto
```

Further stages of the proof

- Ensuring the red density between X, Y is high enough
- Ensuring that X and Y aren't "used up" too quickly
- Exponential improvements away from the diagonal
- The main result, on the diagonal ($k = \ell$)

Computer Algebra Aspects

Formalising claims about limits

- * Accumulate equalities required by each theorem, e.g. $\ell \ge (6/\mu)^{12/5}$ or $\frac{2}{\ell} \le (\mu - 2/\ell)((5/4)^{1/\lceil \ell^{1/4} \rceil} - 1)$
- Check them out by plotting in Maple
- ... then prove that they actually hold in the limit
- For the base cases, use the proof method real_asymp

Limit claims either local to the theorem

let ?Big = " λ l. m_of l \geq 12 \wedge l \geq (6/ μ) powr (12/5) \wedge l \geq 15 \wedge 1 \leq 5/4 * exp (- ((b_of l)^2) / ((μ - 2/l) * m_of l)) \wedge μ > 2/l \wedge 2/l \leq (μ - 2/l) * ((5/4) powr (1/b_of l) - 1)" have big_enough_l: " $\forall \infty$ l. ?Big l" unfolding m of def b of def using assms by (intro eventually conj; real asymp)

Or separate from the theorem

Landau symbols in the proofs

Many formulas such as $|Y| \ge 2^{o(k)}p_0^{s+t} \cdot |Y_0|$

Quite a few different Landau symbol occurrences, but mostly o(k)

I preferred making these functions explicit

Proving $\prod_{i \in \mathscr{D}} \frac{|X_i|}{|X_{i-1}|} = 2^{o(k)}$

A proof using exact calculations

Since $\delta = \min\{1/200, \gamma/20\}$, to deduce that $t \ge 2k/3$ it now suffices to check that¹¹

$$\left(1 - \frac{1}{200\gamma}\right) \left(1 + \frac{1}{e(1-\gamma)}\right)^{-1} \ge \left(1 - \frac{1}{40}\right) \left(1 + \frac{5}{4e}\right)^{-1} > 0.667 > \frac{2}{3}$$
(47)

for all $1/10 \leq \gamma \leq 1/5$, and that

define c where "c $\equiv \lambda x::$ real. 1 + 1 / (exp 1 * (1-x))" define f47 where "f47 $\equiv \lambda x$. (1 - 1/(200*x)) * inverse (c x)" have "concave_on {1/10..1/5} f47" [46 lines] moreover have "f47(1/10) > 0.667" unfolding f47_def c_def by (approximation 15) moreover have "f47(1/5) > 0.667" unfolding f47_def c_def by (approximation 15) ultimately have 47: "f47 x > 0.667" if "x \in {1/10..1/5}" for x using concave_on_ge_min that by fastforce

Proving Lemma A.4

```
lemma A4:
    assumes "y ∈ {0.341..3/4}"
    shows "f2 (x_of y) y ≤ 2 - 1/2^11"
    unfolding f2_def f1_def x_of_def H_def
    using assms by (approximation 18 splitting: y = 13)
```

```
goal (1 subgoal):
1. 3 * y / 5 + 5454 / 10 ^ 4 + y +
   (2 - (3 * y / 5 + 5454 / 10 ^ 4)) *
   (- (1 / (2 - (3 * y / 5 + 5454 / 10 ^ 4))) *
    log 2 (1 / (2 - (3 * y / 5 + 5454 / 10 ^ 4))) -
      (1 - 1 / (2 - (3 * y / 5 + 5454 / 10 ^ 4))) *
      log 2 (1 - 1 / (2 - (3 * y / 5 + 5454 / 10 ^ 4))) *
      log 2 (1 - 1 / (2 - (3 * y / 5 + 5454 / 10 ^ 4))) -
      1 / (40 * ln 2) *
      ((1 - (3 * y / 5 + 5454 / 10 ^ 4)) / (2 - (3 * y / 5 + 5454 / 10 ^ 4)))
      < 2 - 1 / 2 ^ 11</pre>
```

Conclusions

- Some proofs really do need computer algebra or exact arithmetic
- The approximation and real_asymp proof methods are fast and powerful
- Differentiation by pure inference is easy, if a hack
- This proof is incredibly difficult

```
text <Main theorem 1.1: the exponent is approximately 3.9987>
theorem Main 1 1:
  obtains \varepsilon::real where "\varepsilon>0" "\forall^{\infty}k. RN k k \leq (4-\varepsilon)^k"
proof
  let ?ε = "0.00134::real"
  have "\forall^{\infty}k. k>0 \land log 2 (RN k k) / k \leq 2 - delta'"
    unfolding eventually_conj_iff using Aux 1 1 eventually gt at top by blast
  then have "\forall^{\infty}k. RN k k \leq (2 powr (2-delta')) ^ k"
  proof (eventually elim)
    case (elim k)
    then have "log 2 (RN k k) \leq (2-delta') * k"
      by (meson of nat 0 less iff pos divide le eq)
    then have "RN k k \leq 2 powr ((2-delta') * k)"
      by (smt (verit, best) Transcendental.log le iff powr ge zero)
    then show "RN k k \leq (2 powr (2-delta')) ^ k"
      by (simp add: mult.commute powr power)
  qed
  moreover have "2 powr (2-delta') \leq 4 - ?\varepsilon"
    unfolding delta'_def by (approximation 25)
  ultimately show "\forall^{\infty}k. real (RN k k) \leq (4-?\varepsilon) ^ k"
    by (smt (verit) power mono powr ge zero eventually mono)
qed auto
```

The whole development is 11 K lines and runs in under 9 minutes. Formalisation took 251 days.

Many thanks to Mantas Baksys, Manuel Eberl, Simon Griffiths, Fabian Immler, Bhavik Mehta and Andrew Thomason

(If you want to understand the actual proof, please see Bhavik's *Lean Together* talk on the **leanprover community** YouTube channel)