How to Automatise Proofs of Operator Statements: Moore-Penrose Inverse – a Case Study

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HANDBOOK OF LINEAR ALGEBRA

SECOND EDITION

$$\begin{bmatrix} 2 & 2 & 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 4 & 6 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \\ 0 & 0 & 2 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Edited by

Leslie Hogben



Definitions:

A Moore-Penrose pseudo-inverse of a matrix $A \in \mathbb{C}^{m \times n}$ is a matrix $A^{\dagger} \in \mathbb{C}^{n \times m}$ that satisfies the following four Penrose conditions:

$$AA^{\dagger}A = A$$
: $A^{\dagger}AA^{\dagger} = A^{\dagger}$: $(AA^{\dagger})^* = AA^{\dagger}$: $(A^{\dagger}A)^* = A^{\dagger}A$.

Facts:

All the following facts except those with a specific reference can be found in [Gra83, pp. 105-141] or [RM71, pp. 44-67].

- Every A ∈ C^{m×n} has a unique pseudo-inverse A[†].
 - If A ∈ R^{m×n}, then A[†] is real.
 - 3. If $A \in \mathbb{C}^{m \times n}$ of rank r has a full rank decomposition A = BC, where $B \in \mathbb{C}^{m \times r}$ and $C \in \mathbb{C}^{r \times n}$, then A^{\dagger} can be evaluated using $A^{\dagger} = C^*(B^*AC^*)^{-1}B^*$.
- LH95, p. 38 If A ∈ C^{m×n} of rank r < min{m, n} has an SVD A = UΣV*, then its pseudo-inverse is $A^{\dagger} = V \Sigma^{\dagger} U^*$, where

$$\Sigma^{\dagger} = \text{diag}(1/\sigma_1, \dots, 1/\sigma_r, 0, \dots, 0) \in \mathbb{R}^{n \times m}$$
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5. [Hig96, p. 412] The pseudo-inverse A^{\dagger} of $A \in F^{m \times n}$ ($F = \mathbb{C}$ or \mathbb{R}) solves the minimization problem

$$\min_{X \in F^{n \times m}} ||AX - I_m||_F^2.$$

6. $\mathbf{0}_{mn}^{\dagger} = \mathbf{0}_{nm}$ and $J_{mn}^{\dagger} = \frac{1}{mn}J_{nm}$, where $\mathbf{0}_{mn} \in \mathbb{C}^{m \times n}$ is the all 0s matrix and $J_{mn} \in$ $\mathbb{C}^{m \times n}$ is the all 1s matrix.

- 7. If $\mathbf{x} \neq \mathbf{0}$, $\mathbf{y} \neq \mathbf{0}$, then $(\mathbf{x}\mathbf{y}^*)^{\dagger} = \frac{\mathbf{y}\mathbf{x}^*}{\|\mathbf{x}\|^2 \|\mathbf{y}\|^2}$.
- 8. If $\mathbf{x} \neq \mathbf{0}$, then $\mathbf{x}^{\dagger} = \frac{\mathbf{x}^*}{\|\mathbf{x}\|^2}$.
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Then

(a) $(\alpha A)^{\dagger} = \alpha^{\dagger} A^{\dagger}$.

(b) $(\operatorname{diag}(\beta_1, \beta_2, \dots, \beta_n))^{\dagger} = \operatorname{diag}(\beta_1^{\dagger}, \beta_2^{\dagger}, \dots, \beta_n^{\dagger})$.

- 10. $(A^{\dagger})^* = (A^*)^{\dagger}$: $(A^{\dagger})^{\dagger} = A$.
- If A is a nonsingular square matrix, then A[†] = A⁻¹.
- If U has orthonormal columns or orthonormal rows, then U[†] = U*.
- 13. If $A = A^*$ and $A = A^2$, then $A^{\dagger} = A$.
- A[†] = A* if and only if A*A is idempotent.
- If A is normal and k is a positive integer, then AA[†] = A[†]A and (A^k)[†] = (A[†])^k.
- If U ∈ C^{m×n} is of rank n and satisfies U[†] = U*, then U has orthonormal columns. If U ∈ C^{m×m} and V ∈ C^{n×n} are unitary matrices, then (UAV)[†] = V*A[†]U*.
- 18. $A^{\dagger} = (A^*A)^{\dagger}A^* = A^*(AA^*)^{\dagger}$. In particular,
 - (a) if A ∈ C^{m×n} (m > n) has full rank n, then A[†] = (A*A)⁻¹A*;
- (b) if A ∈ C^{m×n} (m ≤ n) has full rank m, then A[†] = A*(AA*)⁻¹.
- 19. Let $A \in \mathbb{C}^{m \times n}$. Then

- (a) A[†]A, AA[†], I_n − A[†]A, and I_m − AA[†] are orthogonal projections.
 - (b) $rank(A) = rank(A^{\dagger}) = rank(AA^{\dagger}) = rank(A^{\dagger}A)$.
 - (c) $rank(I_n A^{\dagger}A) = n rank(A)$.
 - (d) $\operatorname{rank}(I_m AA^{\dagger}) = m \operatorname{rank}(A)$.

Inner Product Spaces, Orthogonal Projection, Least Squares

- 20. $AA^{\dagger} = \text{Proj}_{\text{range}(A)}$; $A^{\dagger}A = \text{Proj}_{\text{range}(A)}$.
- 21. Suppose that $A \in F^{m \times n}$, where $F = \mathbb{C}$ or \mathbb{R} . Then
 - (a) range(A) = range(AA*) = range(AA†).
 - (b) $range(A^{\dagger}) = range(A^*) = range(A^*A) = range(A^{\dagger}A)$.

 - (c) ker(A) = ker(A*A) = ker(A†A).
 - (d) ker(A[†]) = ker(A*) = ker(AA*) = ker(AA[†]).
 - (e) range(A[†]A) ⊕ ker(A[†]A) = Fⁿ.
- (f) range(AA[†]) ⊕ ker(AA[†]) = F^m.
- 22. If $A = A_1 + A_2 + \cdots + A_k$, $A^*A_i = 0$, and $A_iA^* = 0$, for all $i, i = 1, \dots, k, i \neq i$. then $A^{\dagger} = A_1^{\dagger} + A_2^{\dagger} + \cdots + A_n^{\dagger}$.
- 23. If A is an $m \times r$ matrix of rank r and B is an $r \times n$ matrix of rank r, then $(AB)^{\dagger} = B^{\dagger}A^{\dagger}$.
- 24. $(A^*A)^{\dagger} = A^{\dagger}(A^*)^{\dagger}$: $(AA^*)^{\dagger} = (A^*)^{\dagger}A^{\dagger}$.
- [Gre66] Each one of the following conditions is necessary and sufficient for (AB)[†] =
 - (a) range(BB*A*) ⊂ range(A*) and range(A*AB) ⊂ range(B).
 - (b) A[†]ABB* and A*ABB[†] are both Hermitian matrices.
 - (c) $A^{\dagger}ABB^*A^* = BB^*A^*$ and $BB^{\dagger}A^*AB = A^*AB$
 - (d) $A^{\dagger}ABB^*A^*ABB^{\dagger} = BB^*A^*A$.
 - (e) A[†]AB = B(AB)[†]AB and BB[†]A* = A*AB(AB)[†].
- 26. $(A \otimes B)^{\dagger} = A^{\dagger} \otimes B^{\dagger}$, where \otimes denotes the Kronecker product.
- 27. $A^{\dagger} = \lim_{\alpha \to 0} A^{*}(\alpha I + AA^{*})^{-1} = \lim_{\alpha \to 0} (\alpha I + A^{*}A)^{-1}A^{*}$.

$$28. \ A^{\dagger} = \sum^{\infty} A^* (I + AA^*)^{-j} = \sum^{\infty} (I + A^*A)^{-j} A^*.$$

- 29. (Continuity of pseudo-inverse) Suppose that $A \in F^{m \times n}$ and $E \in F^{m \times n}$, where F = \mathbb{C} or \mathbb{R} . Then $\lim_{t \to \infty} (A + E)^{\dagger} = A^{\dagger}$ if and only if there is $\epsilon > 0$ such that $\operatorname{rank}(A + E) =$ rank(A) when $||E||_2 < \epsilon$.
- 30. Let $A \in \mathbb{C}^{m \times n}$ be of rank r where $0 < r < \min\{m, n\}$. Suppose that A can be partitioned as

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

where $A_{11} \in \mathbb{C}^{r \times r}$ and $rank(A_{11}) = r$. Then

$$A^{\dagger} = \begin{bmatrix} A_{11}^* X A_{11}^* & A_{11}^* X A_{21}^* \\ A_{12}^* X A_{11}^* & A_{12}^* X A_{21}^* \end{bmatrix}$$
,

where

$$X = (A_{11}A_{11}^* + A_{12}A_{12}^*)^{-1}A_{11}(A_{11}^*A_{11} + A_{21}^*A_{21})^{-1}.$$

Theory

- Model linear operators by noncomm. polynomials
- Correctness of first-order operator statements

nc ideal membership

- Approach is complete
 - → Semi-decision procedure

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Software

- SAGEMATH package operator_gb*
- Noncomm. Gröbner bases
- Certified nc ideal membership
- Noncomm. ideal arithmetic
- Dedicated methods for proving operator statements

*available at https://github.com/ ClemensHofstadler/operator_gb

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Automated proofs of operator statements

Noncommutative polynomials
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 elements in free algebra $\mathbb{Z}\langle X \rangle$
$$= \sum_{i=1}^d c_i \cdot x_{i,1} \dots x_{i,k_i}$$

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$$\text{Multiplication} = \text{ Concatenation of words}$$

$$(x_1 \dots x_k) \cdot (x_1' \dots x_l') = x_1 \dots x_k x_1' \dots x_l'$$

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Two-sided ideals For
$$f_1, \ldots, f_r \in \mathbb{Z}\langle X \rangle$$

$$(f_1, \dots, f_r) = \left\{ \sum_i \sum_j \alpha_{i,j} \cdot f_i \cdot b_{i,j} \mid \alpha_{i,j}, b_{i,j} \in \mathbb{Z}\langle X \rangle \right\}$$

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Fact Ideal membership problem $f \in (f_1, ..., f_r)$ is semi-decidable (e.g., using Gröbner bases)

Operators

• 0, a, b, c, ...
•
$$s + t$$
, $s \cdot t$, $f(t_1, \ldots, t_n)$

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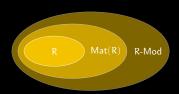


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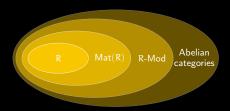


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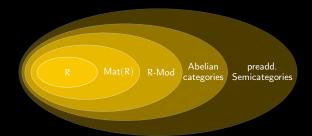


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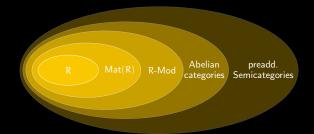
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Linearity = abelian (partial) addition + assoc. (partial) mult. + dist.

Operator statements

$$\mathbf{s} = \mathbf{t}, \quad \neg \, \phi, \quad (\phi \wedge \psi), \quad (\phi \vee \psi), \quad (\phi \Rightarrow \psi), \quad \exists \, \mathbf{x} : \phi, \quad \forall \, \mathbf{x} : \phi$$



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- Fact: Determining universal truth is not decidable ⇒ Algorithm that terminates on all inputs cannot exist
- Best we can hope for: (effective) semi-decision procedure \rightarrow Can be obtained using computer algebra

Idea Translate universal truth of formula into polynomial predicate

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Quasi-identities

 Classical case of quasi-identities well studied (Helton, Stankus, Wavrik '98, Schmitz, Levandovskyy '20, Raab, Regensburger, Hossein Poor '21)

$$\forall \mathbf{X} : \bigwedge_{j=1}^{m} A_{j} = B_{j} \Rightarrow \mathbf{P} = \mathbf{Q}$$

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Strategy

• Interpret each operator as polynomial in $\mathbb{Z}\langle \mathbf{X}\rangle$ and reformulate each identity L=R as polynomial L-R

e.g.,
$$AB = BA \quad \rightsquigarrow \quad ab - ba \in \mathbb{Z}\langle a, b \rangle$$

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Theorem

$$\forall \mathbf{X} : \bigwedge_{j=1}^{m} A_j = B_j \Rightarrow \mathbf{P} = \mathbf{Q} \quad \text{iff} \quad \mathbf{p} - \mathbf{q} \in (a_1 - b_1, \dots, a_m - b_m)$$

Recall: B is Moore-Penrose inverse of A if

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Claim If B and C satisfy these identities, then B = C

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```
sage: from operator_gb import *
sage: assumptions = [a*b*a - a,...]
sage: certify(assumptions, b - c)
```

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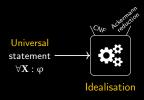
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Proof Using our software package operator_gb...

- Software produces cofactor representation (= certificate for ideal membership)
- Cofactor representation is algebraic proof requiring only linearity
 - ⇒ Statement is proven in all settings where linearity holds

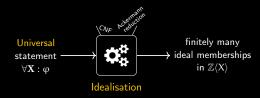
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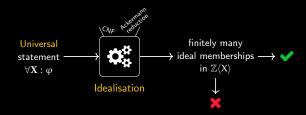
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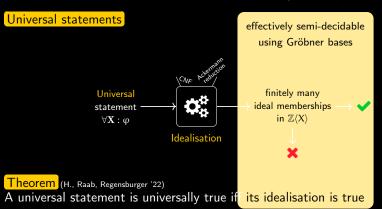
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Theorem (H., Raab, Regensburger '22)

A universal statement is universally true iff its idealisation is true

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- 18. $A^{\dagger} = (A^*A)^{\dagger}A^* = A^*(AA^*)^{\dagger}$. In particular, (a) if A ∈ C^{m×n} (m > n) has full rank n, then A[†] = (A*A)⁻¹A*;
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Inner Product Spaces, Orthogonal Projection, Least Squares

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- 23. If A is an $m \times r$ matrix of rank r and B is an $r \times n$ matrix of rank r, then $(AB)^{\dagger} = B^{\dagger}A^{\dagger}$. **24.** $(A^*A)^{\dagger} = A^{\dagger}(A^*)^{\dagger}$: $(AA^*)^{\dagger} = (A^*)^{\dagger}A^{\dagger}$.
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where $A_{11} \in \mathbb{C}^{r \times r}$ and $rank(A_{11}) = r$. Then

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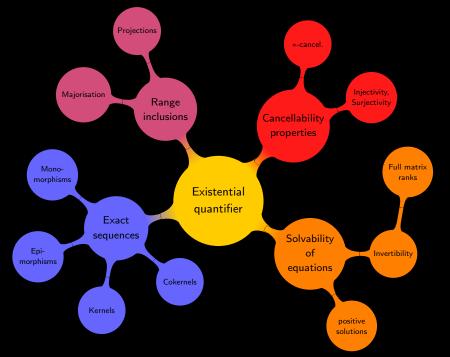
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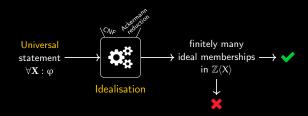
- Enumerating all possible expressions is hopeless
- ullet Requires good heuristics o provided by computer algebra
- Several heuristics implemented in operator_gb
 (ansatz, variable elimination, ideal/subalgebra intersections,...)

Existential quantifier



Idea Translate universal truth of formula into polynomial predicate

Universal statements

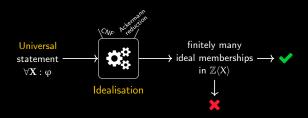


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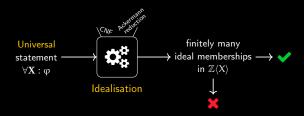


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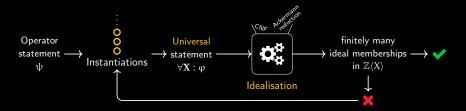


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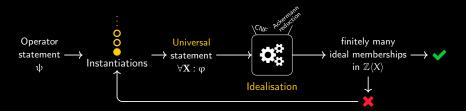


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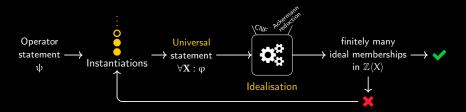


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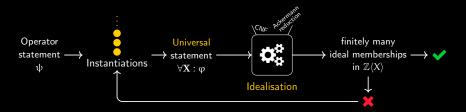


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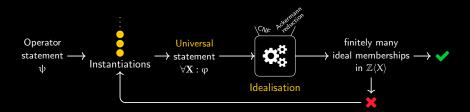


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An operator statement is universally true iff the procedure terminates and returns \checkmark

Definitions:

A Moore-Penrose pseudo-inverse of a matrix $A \in \mathbb{C}^{m \times n}$ is a matrix $A^{\dagger} \in \mathbb{C}^{n \times m}$ that satisfies the following four Penrose conditions:

$$AA^{\dagger}A = A$$
: $A^{\dagger}AA^{\dagger} = A^{\dagger}$: $(AA^{\dagger})^* = AA^{\dagger}$: $(A^{\dagger}A)^* = A^{\dagger}A$.

Facts:

All the following facts except those with a specific reference can be found in [Gra83, pp. 105-141] or [RM71, pp. 44-67].

- ✓ Every A ∈ C^{m×n} has a unique pseudo-inverse A[†].
- If A ∈ R^{m×n}, then A[†] is real.
- \mathcal{J} . If $A \in \mathbb{C}^{m \times n}$ of rank r has a full rank decomposition A = BC, where $B \in \mathbb{C}^{m \times r}$ and $C \in \mathbb{C}^{r \times n}$, then A^{\dagger} can be evaluated using $A^{\dagger} = C^*(B^*AC^*)^{-1}B^*$.
- √ [LH95, p. 38] If A ∈ C^{m×n} of rank r < min{m, n} has an SVD A = UΣV*, then its
 </p> pseudo-inverse is $A^{\dagger} = V \Sigma^{\dagger} U^*$, where

$$\Sigma^{\dagger} = \text{diag}(1/\sigma_1, \dots, 1/\sigma_r, 0, \dots, 0) \in \mathbb{R}^{n \times m}$$
.

 $\fill Hig96$, p. 412 The pseudo-inverse A^{\dagger} of $A \in F^{m \times n}$ ($F = \mathbb{C}$ or \mathbb{R}) solves the minimization problem

$$\min_{X \in F^{n \times m}} ||AX - I_m||_F^2.$$

 \mathbf{G} . $\mathbf{O}_{mn}^{\dagger} = \mathbf{O}_{nm}$ and $J_{mn}^{\dagger} = \frac{1}{mn} J_{nm}$, where $\mathbf{O}_{mn} \in \mathbb{C}^{m \times n}$ is the all 0s matrix and $J_{mn} \in \mathbb{C}^{m \times n}$ $\mathbb{C}^{m \times n}$ is the all 1s matrix.

- \checkmark . If $\mathbf{x} \neq \mathbf{0}$, $\mathbf{y} \neq \mathbf{0}$, then $(\mathbf{x}\mathbf{y}^*)^{\dagger} = \frac{\mathbf{y}\mathbf{x}^*}{\|\mathbf{y}\|^2 \|\mathbf{y}\|^2}$.
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Then

- $(\alpha A)^{\dagger} = \alpha^{\dagger} A^{\dagger}$.
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- M. If A is a nonsingular square matrix, then A[†] = A⁻¹.
- If U has orthonormal columns or orthonormal rows, then U[†] = U^{*}.
- N. If $A = A^*$ and $A = A^2$, then $A^{\dagger} = A$.
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- If A is normal and k is a positive integer, then AA[†] = A[†]A and (A^k)[†] = (A[†])^k. M. If U ∈ C^{m×n} is of rank n and satisfies U[†] = U*, then U has orthonormal columns.
- W. If $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times n}$ are unitary matrices, then $(UAV)^{\dagger} = V^*A^{\dagger}U^*$. 18. $A^{\dagger} = (A^*A)^{\dagger}A^* = A^*(AA^*)^{\dagger}$. In particular,
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Inner Product Spaces, Orthogonal Projection, Least Squares

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