Validating Mathematical Structures

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Abstract. With regard to formalizing mathematics in proof assistants, the hierarchy of mathematical structure that allows for the sharing of notations and theories, and makes subtyping of structures implicit, is a key ingredient of infrastructure to support the users. The packed classes method is a generic design pattern to define and combine mathematical structures in a dependent type theory with records. The Coq proof assistant has mechanisms to enable automated structure inference and subtyping with packed classes; that is, implicit coercions and canonical structures. In this paper, we identify the invariants of hierarchies that ensure the modularity of reasoning and the predictability of inference with packed classes, propose checking tools for those invariants, and show that our tools significantly improve the development process of Mathematical Components, a formalized mathematics library for Coq.

1 Introduction

With regard to formalizing mathematics in proof assistants, the hierarchy of mathematical structure is a key ingredient of infrastructure to support the users, e.g., [18,40,25][10, Chap. 2 and 4][20, Sect. 3][30, Chap. 5][43, Sect. 4]. Since mathematical structures have inheritance/subtyping such that “a field is a ring, a ring is a group, and a group is a monoid”, it is usual practice in mathematics to reuse notations, definitions, and theories of superclasses implicitly to reason about a subclass; thus, it is desirable to have mechanisms supporting the sharing of notations and theories to avoid repeating similar definitions and proofs, and automated inference to make subtyping of structures implicit.

The packed classes method [17,16] is a generic design pattern to define and combine mathematical structures in a dependent type theory with records, which supports multiple inheritance, and maximal sharing of definitions, notations, and theories. In the Coq proof assistant [41], the implicit coercion [32,33,41] and canonical structure [33,26,41] mechanisms enable subtyping and automated inference of structures. Compared to type classes [39,22] based approaches, the packed classes method is robust, and its inference is efficient and predictable (Sect. 8). The success of the packed classes method in formalized mathematics can be seen in the Mathematical Components library [42], the Coquelicot library [7], and in particular, the formal proof of the Odd Order Theorem [20]; on the other hand, it has also been successfully applied for program verification tasks, e.g., a hierarchy of monadic effects [2] and a hierarchy of partial commutative monoids [28] for Fine-grained Concurrent Separation Logic [38].
In spite of its success, the packed classes method is hard to master for library designers and requires substantial amount of work. For instance, the strict application of packed classes requires to define quadratically many implicit coercions and canonical projections for the number of structures. To give some figures, the Mathematical Components library 1.10.0 uses this method ubiquitously to define 51 mathematical structures depicted in Fig. 1, and declares 554 implicit coercions and 746 canonical projections to implement their inheritance. Moreover, defining new intermediate structures between existing ones requires to fix their subclasses and their inheritance accordingly; thus, it can be a challenging task.

In this paper, we identify the invariants of hierarchies in packed classes concerning implicit coercions and canonical structures, and propose tools to support its large-scale deployment by checking those invariants. The invariant concerning implicit coercions ensures the modularity of reasoning with packed classes, is generally useful in a dependent type theory with inheritance beyond packed classes and the Coq system, and was proposed before as a coherence of inheritance graphs [6]. In Sect. 3, we propose a new coherence checking mechanism implemented in Coq. The invariant concerning canonical structures (Sect. 4) ensures the predictability of structure inference. In Sect. 5, we define a simplified model of hierarchies, inheritances, and structure inference; then show a metatheorem that formally states the predictability of structure inference. Sect. 6 presents an external tool that checks this invariant and generates an exhaustive set of assertions for structure inference, whose generated assertions can be checked inside Coq. Sect. 7 demonstrates that our tools can detect and help to fix inheritance bugs in a large-scale development, the Mathematical Components library 1.7.0, and also shows that our tools help the developers of and contributors to Mathematical Components to extend the hierarchy with new structures.

Our running example for Sect. 2, 4, 6, formalization for Sect. 5, and evaluation script for Sect. 7 are available at [36].
2 Packed classes

This section reviews the packed classes method [17,16] by example except for the use of canonical structures. Our example is a minimal hierarchy with multiple inheritance consisting of the following four algebraic structures (Fig. 2):

**Additive monoids** \((A, +, 0)\): Monoids have an associative binary operation \(+\) on \(A\) and an identity element \(0\) of \(A\) with respect to addition.

**Semirings** \((A, +, 0, \times, 1)\): Semirings have the monoid axioms, commutativity of addition, multiplication, and \(1\). Multiplication \(\times\) is an associative binary operation on \(A\) that is left and right distributive over addition. \(0\) and \(1\) are absorbing and identity elements with respect to multiplication respectively.

**Additive groups** \((A, +, 0, -)\): Groups have the monoid axioms and the unary operation \(-\) on \(A\). \(-x\) is the additive inverse of \(x\) for any \(x \in A\).

**Rings** \((A, +, 0, -, \times, 1)\): Rings have all the monoid, semiring, and group axioms, and have no extra axioms.

Here we start with defining the base class, namely the **Monoid** structure.

```lean
Module Monoid.

Record mixin_of (A : Type) := Mixin { 
  zero : A; add : A → A → A; 
  addA : associative add; add0x : left_id zero add; addx0 : right_id zero add }.

Record class_of (A : Type) := Class { mixin : mixin_of A }.

Structure type := Pack { sort : Type; class : class_of sort }.

End Monoid.
```

The above definitions are enclosed by the **Monoid** module and force users to write the qualified names such as **Monoid.type**; thus, we can reuse the same name of records, their constructors, and constants for other structures to indicate their roles. For each structure, we define the **mixin**, **class**, and **type** records. The monoid mixin (line 3) is the set of operations and axioms introduced by the **Monoid** structure, that is, \(0\), \(+\), and their axioms, which are expressed by definitions **associative**, **left_id**, and **right_id** taken from **Mathematical Components** (see Appendix A for details). The monoid class (line 7) is the set of all mixins of
superclasses of the Monoid structure (including itself), which is identical with the mixin record here. The type record (line 9) is the interface of the structure that bundles a carrier of type Type and its class instance. We fix the type of carriers to Type in our examples; thus, the first field of the type record and the type argument of the class_of record should be Type for any structure. In general, it can be other types, e.g., Type → Type in the hierarchy of monads [2].

Mixins and classes are internal definitions to declare mathematical structures; in contrast, Monoid.type is the interface of the monoid structure to reason about monoids. For this reason, we lift zero, add, and their axioms from projections for Monoid.mixin_of to definitions and lemmas for Monoid.type as follows.

Definition zero {A : Monoid.type} : Monoid.sort A :=
  Monoid.zero _ (Monoid.mixin _ (Monoid.class A)).

Definition add {A : Monoid.type} : 
  Monoid.sort A → Monoid.sort A → Monoid.sort A :=
  Monoid.add _ (Monoid.mixin _ (Monoid.class A)).

Lemma addA {A : Monoid.type} : associative (@add A).

Lemma add0x {A : Monoid.type} : left_id (@zero A) (@add A).

Lemma addx0 {A : Monoid.type} : right_id (@zero A) (@add A).

The curly brackets used for A mark it as an implicit argument; in contrast, @ is the explicit application symbol that deactivates the hiding of implicit arguments.

Since a monoid instance A : Monoid.type can be seen as a type equipped with monoid axioms, it is natural to declare Monoid.sort as an implicit coercion. The types of zero can be written and shown as ∀ A : Monoid.type, A rather than ∀ A : Monoid.type, Monoid.sort A thanks to this implicit coercion.

Coercion Monoid.sort : Monoid.type >→ Sortclass.

Next we define the Semiring structure. Since the semiring axioms interact with the monoid operators, the mixin_of record of semirings should take Monoid.type rather than Type as its argument.

Module Semiring.

Record mixin_of (A : Monoid.type) := Mixin {
  one : A; mul : A → A → A;
  addC : commutative (@add A);
  mulA : associative mul;
  mulix : left_id one mul;
  mul1x : right_id one mul;
  mulDl : left_distributive mul add;
  mulDr : right_distributive mul add;
  mul0x : left_zero zero mul;
  mulx0 : right_zero zero mul }.

Record class_of {A : Type} :=
  Class { base : Monoid.class_of A; mixin : mixin_of (Monoid.Pack A base) }.

Structure type := Pack { sort : Type; class : class_of sort }.

The semiring structure should inherit from the monoid structure; thus, we can express a canonical way to construct a monoid from a semiring as follows.

Local Definition monoidType (cT : type) : Monoid.type :=
  Monoid.Pack (sort cT) (base _ (class cT)).

End Semiring.

By following the above method, we declare Semiring.sort as an implicit coercion, and then lift mul, one, and the semiring axioms from projections for the mixin to definitions for Semiring.type.
Coercion Semiring.sort : Semiring.type >>> Sortclass.
Definition one {A : Semiring.type} : A := Semiring.one _ (Semiring.mixin _ (Semiring.class A)).
Definition mul {A : Semiring.type} : A → A → A := Semiring.mul _ (Semiring.mixin _ (Semiring.class A)).
Lemma addC {A : Semiring.type} : commutative (@add (Semiring.monoidType A)).
...

In the statement of the first semiring axiom addC, we needed to explicitly write Semiring.monoidType A to get the Monoid.type instance for A : Semiring.type. Fortunately, we can omit it by declaring Semiring.monoidType is an implicit coercion. In general, for a structure S inheriting from some other structure(s), we define the functions from S to its all the superclasses and declare them as implicit coercions as follows.

Coercion Semiring.monoidType : Semiring.type >>> Monoid.type.

The Group structure is monoids extended with an additive inverse. By following the above methodology, it can be defined as follows.

Module Group.

Record mixin_of (A : Monoid.type) := Mixin {
  opp : A → A;
  addNx : left_inverse zero opp add; addxN : right_inverse zero opp add }.

Record class_of (A : Type) := Class { base : Monoid.class_of A; mixin : mixin_of (Monoid.Pack A base) }.

Structure type := Pack { sort : Type; class : class_of sort }.

Local Definition monoidType (cT : type) : Monoid.type := Monoid.Pack (sort cT) (base _ (class cT)).

End Group.

Coercion Group.sort : Group.type >>> Sortclass.
Coercion Group.monoidType : Group.type >>> Monoid.type.
Definition opp {A : Group.type} : A → A := Group.opp _ (Group.mixin _ (Group.class A)).
...

The Ring structure can be seen as both groups extended by the semiring axioms and semiring extended by the group axioms. Here we define it in the first sense, but one may define it conversely. Since rings have no extra axioms other than the group and semiring axioms, no further mixin_of record is needed.¹

Module Ring.

Record class_of (A : Type) := Class {
  base : Group.class_of A;
  mixin : Semiring.mixin_of (Monoid.Pack A (Group.base A base)) }.

Structure type := Pack { sort : Type; class : class_of sort }.

¹ One may also define a new structure that inherits from multiple existing classes and have an extra mixin, e.g., defining commutative rings instead of rings in this example, and left algebras lalgType in Mathematical Components.
The ring structure inherits from monoids, groups, and semirings. Here we define implicit coercions from the ring structure to those superclasses.

Local Definition monoidType (cT : type) : Monoid.type :=
  Monoid.Pack (sort cT) (Group.base _ (base _ (class cT))).
Local Definition groupType (cT : type) : Group.type :=
  Group.Pack (sort cT) (base _ (class cT)).
Local Definition semiringType (cT : type) : Semiring.type :=
  Semiring.Pack (sort cT) (Semiring.Class _ (Group.base _ (base _ (class cT)))
  (mixin _ (class cT))).
End Ring.

Coercion Ring.sort : Ring.type >-> Sortclass.
Coercion Ring.monoidType : Ring.type >-> Monoid.type.
Coercion Ring.semiringType : Ring.type >-> Semiring.type.
Coercion Ring.groupType : Ring.type >-> Group.type.

3 Coherence of implicit coercions

This section studies the implicit coercion mechanism of Coq and the coherence [6] of inheritance graphs that ensure the modularity of reasoning with packed classes, and presents the coherence checking mechanism we implemented in Coq. In Appendix B, we study another invariant of hierarchies concerning concrete instances and implicit coercions. Detailed usage of implicit coercions can be found in the reference manual [41, Implicit Coercions], and its typing algorithm is described in [32]. First, we define classes and implicit coercions.

Definition 3.1 (Classes [32, Sect. 3.1][41, Implicit Coercions]). A class with \(n\) parameters is any defined name \(C\) with a type \(\forall (x_1 : T_1) \ldots (x_n : T_n)\), sort where sort is \(S\text{Prop}\), \(\text{Prop}\), \(\text{Set}\), or \(\text{Type}\). Thus a class with parameters is considered as a single class and not as a family of classes. An object of class \(C\) is any term of type \(C t_1 \ldots t_n\).

Definition 3.2 (Implicit coercions). A name \(f\) can be declared as an implicit coercion from a source class \(C\) to a target class \(D\) with \(k\) parameters if the type of \(f\) has the form \(\forall x_1 \ldots x_k (y : C t_1 \ldots t_n), D u_1 \ldots u_m\). We then write \(f : C \implies D\).

An implicit coercion \(f : C \implies D\) can be seen as subtyping \(C \leq D\) and applied to fill type mismatch to a term of class \(C\) placed in a context that expects to have a term of class \(D\). Implicit coercions form an inheritance graph with classes as nodes and coercions as edges, whose path \([f_1; \ldots; f_n]\) where \(f_i : C_i \implies C_{i+1}\) can also be seen as subtyping \(C_1 \leq C_{n+1}\); thus we write \([f_1; \ldots; f_n] : C_1 \implies C_{n+1}\) to indicate \([f_1; \ldots; f_n]\) is an inheritance path from \(C_1\) to \(C_{n+1}\). The Coq system pre-computes those inheritance paths for any pair of source and target classes, and updates to keep them closed under transitivity when a new implicit coercion is declared [32, Sect. 3.3][41, Inheritance Graph]. The coherence of inheritance graphs is defined as follows.

\(^2\) In fact, the target class can also be functions (Funclass) and sorts (Sortclass); that is to say, a function returning functions, types, or propositions can be declared as an implicit coercion. In this paper, we omit these cases to make explanations simple, but our discussion can be generalized to these cases.
Definition 3.3 (Definitional equality [15, Sect. 3.1]). Terms $t_1$ and $t_2$ are said to be definitionally equal or convertible if they are equivalent by βδiζ-reduction and η-expansion. This equality is denoted by the infix symbol $\equiv$.

Definition 3.4 (Coherence [6, Sect. 3.2][32, Sect. 7]). An inheritance graph is coherent if and only if the following two conditions hold.

1. For any circular inheritance path $p : C \rightarrow C$, $px \equiv x$ where $x$ is a fresh variable of class $C$.
2. For any two inheritance paths $p, q : C \rightarrow D$, $px \equiv qx$ where $x$ is a fresh variable of class $C$.

If multiple inheritance paths between the same source and target classes exist, only the oldest one is kept as a valid one in the inheritance graph, and all the others are reported as ambiguous paths and ignored in Coq before our work. We improved this mechanism to report only paths that break the coherence conditions and also to minimize the number of ambiguous paths reported [35,34]. The second condition ensures the modularity of reasoning with packed classes. For example, proving $\forall (R : \text{Ring.type}) (x, y : R), (\neg x) \times y = \neg (x \times y)$ requires to use both $\text{Semiring.monoidType} (\text{Ring.semiringType} R)$ and $\text{Group.monoidType} (\text{Ring.groupType} R)$ implicitly. If those Monoid instances are not definitionally equal, it will prevent us from proving the lemma by reporting type mismatch between $R$ and $R$.

Convertibility checking for inheritance paths consisting of the implicit coercions as in Definition 3.2 requires to construct a function composition of a given inheritance path. One may encode any unification problem to this well-typed term construction problem, that in higher-order case is undecidable [19]. Nevertheless, those inheritance paths that make the convertibility checking undecidable can never be applied as implicit coercions in type inference because they do not respect the uniform inheritance condition.

Definition 3.5 (Uniform inheritance condition [32, Sect. 3.2] [41, Implicit Coercions]). An implicit coercion $f$ between classes $C \rightarrow D$ with $n$ and $m$ parameters respectively is uniform if and only if the type of $f$ has the form

$$\forall (x_1 : A_1) \ldots (x_n : A_n) (x_{n+1} : C x_1 \ldots x_n), D u_1 \ldots u_m.$$ 

Remark 3.1. Names that can be declared as implicit coercions are defined as constants that respect the uniform inheritance condition in [32, Sect. 3.2]. However, the actual implementation of the modern Coq system accepts almost any functions as in Definition 3.2 as coercions.

Saïbi claimed that the uniform inheritance condition “ensures that any coercion can be applied to any object of its source class” [32, Sect. 3.2], but the actual condition ensures more properties. The number and ordering of parameters of a uniform implicit coercion are the same as those of its source class; thus, convertibility checking of uniform implicit coercions $f, g : C \rightarrow D$ does not require any special treatment such as permuting parameters of $f$ and $g$. Moreover, function composition preserves this uniformity, that is, the following lemma holds.
**Lemma 3.1.** For any uniform implicit coercions $f : C \rightarrow D$ and $g : D \rightarrow E$, the function composition of the inheritance path $[f; g] : C \rightarrow E$ is uniform.

**Proof.** Let us assume that $C$, $D$, and $E$ are classes with $n$, $m$, and $k$ parameters respectively, and $f$ and $g$ have the following types:

$$f : \forall (x_1 : T_1) \ldots (x_n : T_n) (x_{n+1} : C x_1 \ldots x_n), D u_1 \ldots u_m,$$

$$g : \forall (y_1 : U_1) \ldots (y_m : U_m) (y_{m+1} : D y_1 \ldots y_m), E v_1 \ldots v_k.$$

Then the function composition of $f$ and $g$ can be defined and typed as follows:

$$g \circ f := \lambda (x_1 : T_1) \ldots (x_n : T_n) (x_{n+1} : C x_1 \ldots x_n), g u_1 \ldots u_m (f x_1 \ldots x_n x_{n+1})$$

$$: \forall (x_1 : T_1) \ldots (x_n : T_n) (x_{n+1} : C x_1 \ldots x_n),$$

$$E (v_1 \{y_1/u_1\} \ldots \{y_m/u_m\}\{y_{m+1}/f x_1 \ldots x_n x_{n+1}\})$$

It should be noted that the terms $u_1, \ldots, u_m$ contain free variables $x_1, \ldots, x_{n+1}$ and we omitted substitutions for them by using the same names for binders in the above definition. Nonetheless, $(g \circ f) : C \rightarrow E$ respects the uniform inheritance condition.\[ ]

In the above definition of the function composition $g \circ f$ of implicit coercions, types of $x_1, \ldots, x_n, x_{n+1}$ and parameters of $g$ can be automatically inferred in **Coq**; thus, it can be abbreviated as follows:

$$g \circ f := \lambda (x_1 : \_ \ldots (x_n : \_)) (x_{n+1} : \_), g \underbrace{\_ \ldots \_}_{m \text{ parameters}} (f x_1 \ldots x_n x_{n+1}).$$

For implicit coercions $f_1 : C_1 \rightarrow C_2, f_2 : C_2 \rightarrow C_3, \ldots, f_n : C_n \rightarrow C_{n+1}$ that have $m_1, m_2, \ldots, m_n$ parameters respectively, the function composition of the inheritance path $[f_1; f_2; \ldots; f_n]$ can be written as follows by applying Lemma 3.1 and the above abbreviation repetitively.

$$f_n \circ \ldots \circ f_2 \circ f_1 := \lambda (x_1 : \_ \ldots (x_{m_1} : \_)) (x_{m_1+1} : \_),$$

$$f_n \underbrace{\_ \ldots \_}_{m_n \text{ parameters}} (f_{m_2} \underbrace{\_ \ldots \_}_{m_2 \text{ parameters}} (f_{m_1} x_1 \ldots x_{m_1} x_{m_1+1}) \ldots).$$

If $f_1, \ldots, f_n$ are uniform, the numbers of their parameters $m_1, \ldots, m_n$ are equal to the numbers of parameters of $C_1, \ldots, C_n$; thus, the type inference algorithm always produces the typed closed term of most general function composition of $f_1, \ldots, f_n$ from the above term. If some of $f_1, \ldots, f_n$ are not uniform, type inference may fail or produce an open term, but if this produces a typed closed term, it is the most general function composition of $f_1, \ldots, f_n$.

Our coherence checking mechanism constructs the function composition of $p : C \rightarrow C$ and compare it with the identity function of class $C$ to check the first condition; and also constructs the function compositions of $p, q : C \rightarrow D$ and performs the conversion test for them to check the second condition.
4 Automated structure inference

This section reviews how the automated structure inference mechanism [26] work in our example and in general. The first example is 0+1, which can also be written as a verbose Gallina term with holes: \texttt{add _ (@zero _)} \texttt{( @one _)}. The left- and right-hand sides of this term can be type-checked without any use of canonical structures as follows:

\begin{verbatim}
?_1 : Monoid.type ⊢ @add ?_1 (@zero ?_1) : Monoid.sort ?_1 → Monoid.sort ?_1,
?_2 : Semiring.type ⊢ @one ?_2 : Semiring.sort ?_2,
\end{verbatim}

where \(?_1\) and \(?_2\) represent unification variables. Type-checking the application of the above terms \texttt{add ?_1 (@zero ?_1) (@one ?_2)} requires to solve a unification problem \texttt{Monoid.sort ?_1 ≡ Semiring.sort ?_2}, which Coq does not know how to solve without hints. By declaring \texttt{Semiring.monoidType : Semiring.type → Monoid.type} as a canonical projection, Coq can be aware of that instantiating \(?_1\) with \texttt{Semiring.monoidType ?_2} is the canonical solution of this unification problem.

The second example is \texttt{−1}, which can also be written as \texttt{@opp _ (@one _)}.

Type-checking their application \texttt{opp ?_3 (@one ?_4)} requires to solve a unification problem \texttt{Group.sort ?_3 ⊢ Semiring.sort ?_4}, which Coq indeed does not know how to solve without hints. Moreover, the group structure and the semiring structure do not inherit from each other; therefore, this case is not an instance of the above criteria to define canonical projections. Nevertheless, this unification problem means that \(?_3\) with \texttt{Semiring.monoidType ?_5} and \texttt{Ring.semiringType ?_5} respectively. Right after defining \texttt{Ring.semiringType}, this unification hint can be defined as follows.
Local Definition semiring_groupType (cT : type) : Group.type :=
  Group.Pack (Semiring.sort (semiringType cT)) (base _ (class cT)).

This definition is definitionally equal to Ring.groupType, but they have the
different head symbols Semiring.sort and Ring.sort respectively in their first
fields Group.sort; thus, the unification hint we need between Group.sort and
Semiring.sort can be synthesized by the following declarations.

Canonical Ring.semiring_groupType.

This unification hint can also be defined conversely as follows. Whichever of
Ring.semiring_groupType and Ring.group_semiringType is acceptable, at
least one of them should be declared.

Local Definition group_semiringType (cT : type) : Semiring.type :=
  Semiring.Pack (Group.sort (groupType cT))
    (Semiring.Class _ (Group.base _ (base _ (class cT)))
     (mixin _ (class cT))).

For any structure $A$ and $B$ that have common (non-strict) subclasses $C$, we
say that $C \in C$ is a join of $A$ and $B$ if $C$ does not inherit from any other structures
in $C$. For example, if we add the structure of commutative rings to the hierarchy
of Sect. 2, the commutative ring structure is a common subclass of the group
and semiring structures, but is not a join of them because the commutative ring
structure inherits from the ring structure which is another common subclass of
them. In general, the join of any two structures must be unique, and we should
declare a canonical projection to infer the join $C$ as the canonical solution of
unification problems of the form $A.sort \equiv B.sort$. For any structures $A$ and $B$ such that $B$ inherits from $A$, $B$ is the join of $A$ and $B$; thus, the first
criteria to define canonical projections is just an instance of the second criteria.

The diagram on the left of Fig. 3 shows a minimal hierarchy that contains
ambiguous joins. If we declare that $C$ (resp. $D$) is the canonical join of $A$ and $B$ in
this hierarchy, it will also be accidentally inferred for a user who wants to reason
about $D$ (resp. $C$). Since neither $C$ nor $D$ does not inherit from each other, inferred
$C$ (resp. $D$) can never be instantiated with $D$ (resp. $C$); therefore, this ambiguity
must be disambiguated as in the diagram on the right of Fig. 3, so that the join
of $A$ and $B$ can be specialized to both $C$ and $D$ afterwards.
5 A simplified formal model of hierarchies

In this section, we define a simplified formal model of hierarchies and show a metatheorem that ensures the predictability of structure inference. First, we define the model of hierarchies and inheritance relations.

Definition 5.1 (Hierarchy and inheritance relations). A hierarchy \( \mathcal{H} \) is a finite set of structures partially ordered by a non-strict inheritance relation \( \leadsto^* \); that is, \( \leadsto^* \) is reflexive, antisymmetric, and transitive. We denote the corresponding strict (irreflexive) inheritance relation by \( \leadsto^+ \). \( A \leadsto^* B \) and \( A \leadsto^+ B \) respectively mean that \( B \) non-strictly and strictly inherits from \( A \).

Definition 5.2 (Common subclasses). The (non-strict) common subclasses of \( A, B \in \mathcal{H} \) are \( C := \{ C \in \mathcal{H} \mid A \leadsto^* C \land B \leadsto^* C \} \). The minimal common subclasses of \( A \) and \( B \) is \( \text{mcs}(A, B) := C \setminus \{ C \in \mathcal{H} \mid \exists C' \in C, C' \leadsto^+ C \} \).

Definition 5.3 (Well-formed hierarchy). A hierarchy \( \mathcal{H} \) is said to be well-formed if the minimal common subclasses of any two structures are unique; that is, \( |\text{mcs}(A, B)| \leq 1 \) for any \( A, B \in \mathcal{H} \).

Definition 5.4 (Extended hierarchy). An extended hierarchy \( \mathcal{H} := \mathcal{H} \cup \{\top\} \) is a hierarchy \( \mathcal{H} \) extended with \( \top \) which means a structure that strictly inherits from all the structures in \( \mathcal{H} \); thus, the inheritance relation is extended as follows:

\[
\begin{align*}
A \leadsto^* \top & \iff \text{true}, \\
\top \leadsto^* B & \iff \text{false} \quad \text{(if } B \neq \top), \\
A \leadsto^* B & \iff A \leadsto^+ B \quad \text{(if } A \neq \top \text{ and } B \neq \top).
\end{align*}
\]

Definition 5.5 (Join). The join is a binary operator on an extended well-formed hierarchy \( \mathcal{H} \), defined as follows:

\[
\text{join}(A, B) = \begin{cases} 
C & \text{(if } A, B \in \mathcal{H} \text{ and } \text{mcs}(A, B) = \{C\}), \\
\top & \text{(otherwise)}.
\end{cases}
\]

We defined the above concepts on hierarchies in Coq by using the structure of partially ordered finite types \texttt{finPOrderType} of the \texttt{mathcomp-finmap} library [12] and proved the following theorem.

Theorem 5.1. The join operator on an extended well-formed hierarchy is associative, commutative, and idempotent; that is, an extended well-formed hierarchy is a join-semilattice.

Proof. See Appendix C. \( \square \)

If the unification algorithm of Coq respects our model of hierarchies and joins in structure inference, Theorem 5.1 indicates that permuting, duplicating, and contracting unification problems do not change the result of inference; thus, it states the predictability of structure inference at a very abstract level.
Validating well-formedness of hierarchies

This section presents a validation mechanism for the well-formedness and the correctness of unification hints that implement the inference of join. We implemented this checking mechanism as an external tool `hierarchy.ml` written in OCaml, which is available as a developers utility of Mathematical Components [42, /etc/utils/hierarchy.ml].

Since a hierarchy must be a finite set of structures (Definition 5.1), Definitions 5.2, 5.5, and 5.3 give us computable (yet inefficient) descriptions of joins and their invariant; in other words, for a given hierarchy $\mathcal{H}$ and any two structures $A, B \in \mathcal{H}$, one may enumerate their minimal common subclasses and check their uniqueness. The `hierarchy.ml` utility extracts the inheritance relation by interacting with `coqtop` and using the Print Canonical Projections command, computes its transitive closure, and then executes Algorithm 1 to check the well-formedness and to generate the exhaustive set of assertions. Algorithm 1 uses the indexed family of strict subclasses $\text{subof}(A) := \{ B \in \mathcal{H} | A \rightarrow^+ B \}$ rather than the inheritance relations for computations. In this algorithm, the enumeration of minimal common subclasses is done by constructing the set of common subclasses $C$, and filtering out $\text{subof}(C)$ from $C$ for every $C \in C$. In this filtering out process, which is written as a foreach statement, we can skip elements already filtered out and do not need to care about ordering of picking up elements, thanks to transitivity.

Algorithm 1 generates the following assertions from the hierarchy of Sect. 2.

\begin{verbatim}
check_join Group.type Group.type Group.type.
check_join Group.type Monoid.type Group.type.
check_join Group.type Ring.type Ring.type.
check_join Group.type Semiring.type Ring.type.
check_join Monoid.type Group.type Group.type.
check_join Monoid.type Monoid.type Monoid.type.
check_join Monoid.type Ring.type Ring.type.
check_join Monoid.type Semiring.type Semiring.type.
check_join Ring.type Group.type Ring.type.
check_join Ring.type Monoid.type Ring.type.
check_join Ring.type Ring.type Ring.type.
check_join Ring.type Semiring.type Ring.type.
check_join Semiring.type Group.type Ring.type.
check_join Semiring.type Monoid.type Semiring.type.
check_join Semiring.type Ring.type Ring.type.
check_join Semiring.type Semiring.type Semiring.type.
\end{verbatim}

An assertion check_join t1 t2 t3 asserts that the join of $t1$ and $t2$ is $t3$, and is implemented as a tactic which fails if the assertion is false. For instance, if we forget to declare $\text{Ring.semiringType}$ as a canonical projection, the assertion of line 12 fails and reports the following error.

There is no join of Ring.type and Semiring.type but is expected to be Ring.type.

One may declare wrong canonical projections that overwrite an existing join. For example, the join of groups and monoids must be groups; however, defining the following canonical projection in the Ring section overwrites this join.

\begin{verbatim}
Local Definition bad_monoid_groupType : Group.type :=
Group.Pack (Monoid.sort monoidType) (base _ class).
\end{verbatim}
Parameters: \( \mathcal{H} \) is the set of all the structures. \( \text{subof} \) is the map from structures to their strict subclasses, which must be transitive:
\[
\forall A, B \in \mathcal{H}, A \in \text{subof}(B) \Rightarrow \text{subof}(A) \subset \text{subof}(B).
\]

Function join\((A, B)\):
\[
C := (\text{subof}(A) \cup \{A\}) \cap (\text{subof}(B) \cup \{B\});
\]
/* \( C \) is the set of all the common subclasses of \( A \) and \( B \). */

foreach \( C \in C \) do \( C \leftarrow C \setminus \text{subof}(C) \);
/* Since \( \text{subof} \) is transitive, removed elements of \( C \) can be skipped in this loop, and the ordering of picking elements from \( C \) does not matter. */
if \( C = \emptyset \) then return \( \top \); /* There is no join of \( A \) and \( B \). */
else if \( C \) is singleton \( \{C\} \) then return \( C \); /* \( C \) is the join of \( A \) and \( B \). */
else fail; /* The join of \( A \) and \( B \) is ambiguous. */

foreach \( A, B \in \mathcal{H} \) do
\[
C := \text{join}(A, B); \text{ if } C \neq \top \text{ then print } \text{"check join } A \ B \ C.";
\]
end

Algorithm 1: Well-formedness checking and assertions generation for unification hints that implement the inference of join.

By declaring \texttt{Ring.bad_monoid_groupType} as a canonical projection, the join of \texttt{Monoid.type} and \texttt{Group.type} is still \texttt{Group.type}, but the join of \texttt{Group.type} and \texttt{Monoid.type} becomes \texttt{Ring.type}, because of asymmetry of the unification mechanism. The assertion of line 2 fails and reports the following error.

The join of \texttt{Group.type} and \texttt{Monoid.type} is \texttt{Ring.type} but is expected to be \texttt{Group.type}.

7 Evaluation

This section reports the results of applying our tools to the \texttt{Mathematical Components} library 1.7.0 and recent development efforts to extend the hierarchy in \texttt{Mathematical Components} with help from our tools. For further details, see Appendix D. \texttt{Mathematical Components 1.7.0} provides the structures depicted in Fig. 1 except \texttt{comAlgType} and \texttt{comUnitAlgType} and lacked a few edges; thus, it has quite a large-scale hierarchy. Our coherence checking mechanism found 11 inconvertible multiple inheritance paths in the \texttt{ssralg} library. Fortunately, those paths concern proof terms and are intended to be irrelevant; thus we can ensure no implicit coercion breaks the modularity of reasoning. Our well-formedness checking tool discovered 7 ambiguous joins, 8 missing canonical projections, and one overwritten join by a wrong declaration of a canonical instance.

The first issue is that inheritance from the \texttt{CountRing} structures to the \texttt{FinRing} structures is not implemented. That missing inheritance introduces 7 ambiguous joins. For instance, \texttt{finZmodType} does not inherit from \texttt{countZmodType} as it should; thus they become ambiguous joins of \texttt{countType} and \texttt{zmodType}. One and 5 out of 8 missing canonical projections should infer \texttt{countClosedFieldType} and \texttt{FinRing} structures, respectively. The other 2 projections are in ordered field (\texttt{numFieldType} and \texttt{realFieldType}) structures.
The second issue is that the following finType instance for extremal_group overwrites the join of finType and countType, which should be finType.

\[
\text{Canonical extremal_group_finType := FinType _ extremal_group_finMixin.}
\]

In this declaration, FinType is a packager [26, Sect. 7] (see Appendix B) that takes a type T and Finite mixin of T as its arguments and construct a finType instance for T by using the canonical countType instance for T. However, if one omits its first argument T with a placeholder as in above, the packager may behave unpredictably as a unification hint. In the above case, the placeholder is instantiated with extremal_group_countType by type inference; thus it wrongly overwrites the join of finType and countType.

Those inheritance bugs were found and fixed with help from the mechanisms we propose; therefore, the later versions of Mathematical Components have no similar issue. Especially, fixing the first issue of missing inheritance from CountRing to FinRing was a difficult task without automated checking tools. The missing inheritance itself was a known issue from before our tooling work, but the sub-hierarchy consisting of the GRing, CountRing, and FinRing structures in Fig. 1 is quite dense; thus, it prevents the library developers from enumerating joins correctly without tools [37].

Our tools also help contributors to Mathematical Components to find inheritance bugs when extending the hierarchy, moreover, improve the development process by reducing the reviewing and maintenance burden, and allow developers and contributors to focus on mathematical contents and other design issues. For instance, Hivert [24] added new structures of commutative algebras and redefined the field extension and splitting field structures to inherit from them. In this extension process, they fixed some inheritance issues with help from us and our well-formedness checking tool; at the same time, we made sure there is no inheritance bug without reviewing the whole boilerplate code of implicit coercions and canonical projections. We ported the order sub-library of the mathcomp-finmap library [12] to Mathematical Components and redefined ordered domain structures [10, Chap. 4] to inherit from ordered types with help from our tools [14]. This refactoring work became approximately 10,000 lines of changes; thus, reducing the reviewing burden was an even more critical issue.

8 Conclusion and related work

This paper has provided a thorough analysis of the packed classes method, introduced two invariants that ensure the modularity of reasoning and the predictability of structure inference, and presented systematic ways to check those invariants. We implemented our invariant checking mechanisms as a part of the Coq system and an external tool bundled with Mathematical Components. Thanks to those tools, many inheritance bugs in Mathematical Components are found and fixed. Its development process has also been improved significantly.

Coq before our work has no coherence checking mechanism. Saïbi [32, Sect. 7] claimed “it is too restrictive in practice” and “it is better to replace conversion by Leibniz equality to compare path coercions because Leibniz equality is a bigger
relation than conversion”. However, most theorem provers based on dependent type theories including Coq are still heavily relying on conversion, particularly in their type checking/inference mechanisms. The coherence should not be relaxed with Leibniz equality; otherwise, the type mismatch problems described in Sect. 3 will recur. With our coherence checking mechanism, users can still declare inconvertible multiple inheritance at their own risk and responsibility, because ambiguous paths messages are implemented as warnings rather than errors. The Lean theorem prover [5,27] has an implicit coercion mechanism based on type class resolution, that allows users to define and use non-uniform implicit coercions; thus, coherence checking can be more difficult. Actually, Lean has no coherence checking mechanism; thus, users get more flexibility with this mechanism but need to be careful by themselves to be coherent.

There are three kinds of approaches to defining mathematical structures in proof assistants: unbundled, semi-bundled, and bundled approaches [43, Sect. 4.1.1]. The unbundled approach uses an interface that is parameterized by carriers and operators, and gathers axioms as its fields, e.g., [40]; in contrast, the semi-bundled approach bundles operators together with axioms as in class of records, but still places carriers as parameters, e.g., [43]. The bundled approach uses an interface that bundles carriers together with operators and axioms, e.g., packed classes and telescopes [26, Sect. 2.3][8,29,18]. The above difference of definitions of interfaces, in particular, whether carriers are bundled or not, leads to the use of different instance resolution and inference mechanisms: type classes [39,22] for the unbundled and semi-bundled approaches, and canonical structures or other unification hint mechanisms for the bundled approach. Researchers have observed unpredictable behaviors [23] and efficiency problems [43, Sect. 4.3][40, Sect. 11] in inference with type classes; in contrast, structure inference with packed classes is predictable, and Theorem 5.1 states this predictability even formally except for concrete instance resolution. Since the resolution of canonical structure in structure inference is made by looking up a table of unification hints indexed by pairs of two head symbols or recursively applying it without backtracking [21, Sect. 2.3], there is no efficiency problem with structure inference. In the unbundled and semi-bundled approaches, a carrier may be associated with multiple classes; thus, inference of join and our work on structure inference (Sect. 4, 5, and 6) are problems specific to the bundled approach. There are a few mechanisms to extend the unification engine of proof assistants other than canonical structures that can implement structure inference for packed classes: unification hints [3] of Lean and Matita [4], and coercions pullback [31]. For any of those cases, our invariants are fundamental properties to implement packed classes and structure inference, but no tests are made yet.

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A Coq references

The following definitions express the basic properties of algebraic operations and constants used in Sect. 2.

Section ssrfun.
Local Set Implicit Arguments.
Variables S T R : Type.

- left_inverse e inv op ↔ inv is a left inverse of op with respect to identity e, i.e., op (inv x) x = e for any x.
- right_inverse e inv op ↔ inv is a right inverse of op with respect to identity e, i.e., op x (inv x) = e for any x.

Definition left_inverse e inv (op : S → T → R) := ∀ x, op (inv x) x = e.
Definition right_inverse e inv (op : S → T → R) := ∀ x, op x (inv x) = e.

- left_id e op ↔ e is a left identity for op, i.e., op e x = x for any x.
- right_id e op ↔ e is a right identity for op, i.e., op x e = x for any x.

Definition left_id e (op : S → T → T) := ∀ x, op e x = x.
Definition right_id e (op : S → S → S) := ∀ x, op x e = x.

- left_zero z op ↔ z is a left absorbing for op, i.e., op z x = z for any x.
- right_zero z op ↔ z is a right absorbing for op, i.e., op x z = z for any x.

Definition left_zero z (op : S → T → S) := ∀ x, op z x = z.
Definition right_zero z (op : S → S → T) := ∀ x, op x z = z.

- left_distributive op add ↔ op is left distributive over add, i.e., op (add x y) z = add (op x z) (op y z) for any x, y, and z.
- right_distributive op add ↔ op is right distributive over add, i.e., op x (add y z) = add (op x y) (op x z) for any x, y, and z.

Definition left_distributive (op : S → T → S) add := ∀ x y z, op (add x y) z = add (op x z) (op y z).
Definition right_distributive (op : S → T → T) add := ∀ x y z, op x (add y z) = add (op x y) (op x z).

- commutative op ↔ op is commutative, i.e., op x y = op y x for any x and y.
- associative op ↔ op is associative, i.e., op x (op y z) = op (op x y) z for any x, y, and z.

Definition commutative (op : S → S → T) := ∀ x y, op x y = op y x.
Definition associative (op : S → S → S) := ∀ x y z, op x (op y z) = op (op x y) z.

End ssrfun.
B The invariant of packed classes concerning concrete instances and implicit coercions

In this appendix, we study the invariant of the packed classes method concerning concrete instances and implicit coercions, that ensures the modularity of reasoning with regard to concrete instances. We also revisit an existing mechanism to construct concrete instances, packagers [26, Sect. 7]. The packager mechanism is originally presented to make instance declarations easier, but also enforces this invariant to concrete instances. We have not made any systematic checking mechanism for this invariant; thus, this appendix does not provide any original results. Nonetheless, practically we do not need to check this invariant thanks to the packager mechanism.

The packed classes method uses canonical structures for two purposes: structure inference (Sect. 4) and canonical instances declaration for concrete types. For example, one may use the **Canonical** command to declare the canonical instances for binary integers \( \mathbb{Z} \) of the Coq standard library as follows.

```coq
Require Import ZArith.

Definition Z_monoid : Monoid.mixin_of Z :=
  Monoid.Mixin Z 0%Z Z.add Z.add_assoc Z.add_0_l Z.add_0_r.
Canonical Z_monoidType := Monoid.Pack Z (Monoid.Class Z Z_monoid).

Definition Z_semiring : Semiring.mixin_of Z_monoidType :=
  Semiring.Mixin Z_monoidType 1%Z Z.mul Z.add_comm Z.mul_assoc Z.mul_1_l Z.mul_1_r
  Z.mul_add_distr_r Z.mul_add_distr_l Z.mul_0_l Z.mul_0_r.
Canonical Z_semiringType := Semiring.Pack Z (Semiring.Class Z (Monoid.Class Z Z_monoid) Z_semiring).

Definition Z_group : Group.mixin_of Z_monoidType :=
  Group.Mixin Z_monoidType Z.opp Z.add_opp_diag_l Z.add_opp_diag_r.
Canonical Z_groupType :=
  Group.Pack Z (Group.Class Z (Monoid.Class Z Z_monoid) Z_group).

Canonical Z_ringType :=
  Ring.Pack Z (Ring.Class Z (Group.Class Z (Monoid.Class Z Z_monoid) Z_group) Z_semiring).
```

By declaring the first canonical instance \( Z \_monoidType \), the unification algorithm of Coq can solve a unification problem \( \text{Monoid.sort } ?_1 \equiv \mathbb{Z} \) by instantiating \( ?_1 : \text{Monoid.type} \) with \( Z \_monoidType \). Therefore, the type inference algorithm of Coq can instantiate the unification variable \( ?_1 : \text{Monoid.type} \) in a Gallina term \( \text{@add } ?_1 0\%\mathbb{Z} 1\%\mathbb{Z} \) with \( Z \_monoidType \). Other **Canonical** declarations respectively work similarly as unification hints to infer canonical semiring, group, and ring instances for \( \mathbb{Z} \).

The initial motivation to introduce packagers in [26, Sect. 7] was not to repeat the same construction of class instances in canonical instance declarations. For instance, all the above canonical instance declarations have subterm
Monoid.Class Z Z_monoid inside; moreover, Z_ringType is consisting of the monoid, semiring, and group mixins of Z, and thus can be automatically constructed from canonical semiring and group instances in principle. These redundancies exist because the class_of record must be the set of all mixin of superclasses (Sect. 2); in other words, inheritance in packed classes should always be by inclusion rather than construction/theorem. Thanks to these redundancies, canonical concrete instances can always be defined to respect the following proposition, which is the invariant concerning implicit coercions and canonical concrete instances.

**Proposition B.1.** For any structures A and B, and a concrete type T : Type, such that B inherits from A with an implicit coercion B.aType : B.type ℮ A.type and T has the canonical instances T_aType (:= A.Pack T ...) and T_bType (:= B.Pack T ...), the following definitional equation holds:

\[ B.aType \equiv T_aType. \]

By substituting our example of Sect. 2 and their instances for Z into Proposition B.1, the following definitional equations can be obtained:

\[ \text{Semiring.monoidType } Z\text{.semiringType } \equiv \text{Z.monoidType}, \]
\[ \text{Group.monoidType } Z\text{.groupType } \equiv \text{Z.monoidType}, \]
\[ \text{Ring.monoidType } Z\text{.ringType } \equiv \text{Z.monoidType}, \]
\[ \text{Ring.semiringType } Z\text{.ringType } \equiv \text{Z.semiringType}, \]
\[ \text{Ring.groupType } Z\text{.ringType } \equiv \text{Z.groupType}. \]

If Proposition B.1 does not hold, reasonings regarding concrete instances using overloaded operators and lemmas cannot be modular. For example, we cannot reuse definitions and theorems on Z_monoidType to reason about Z_semiringType if equation (1) does not hold. We discuss about this problem in detail in [1, Sect. 3]; also, the same issue and solution has recently been observed in [9, Sect. 3] which uses a bundled type classes based approach.

The packager mechanism provides a way to build a concrete instance of a structure from a concrete type and a mixin of that structure, but mixins of its superclasses are not required. Since the monoid structure has no superclasses, the monoid packager can be defined straightforwardly as the following notation.

**Notation** MonoidType T m := (Monoid.Pack T (Monoid.Class T m)).

The canonical monoid instance for Z can be redefined by using this packager as follows.

**Canonical** Z_monoidType := MonoidType Z Z_monoid.

The semiring packager takes a type and its semiring mixin, fetches the canonical monoid instance for the given type by using a phantom type, and build a semiring instance from them. This packager can be defined as follows by using the infrastructure provided in [26, Sect. 7], except that binders in its [find ...] notations are extended with explicit type annotation.
Definition pack_semiring (T : Type) :=
[find bT : Monoid.type | T ⊑ Monoid.sort bT | "is not an Monoid.type" ]
[find b : Monoid.class_of T | b ⊑ Monoid.class bT ]
  fun m : Semiring.mixin_of (Monoid.Pack T b) =>
  Semiring.Pack T (Semiring.Class T b m).

Notation SemiringType T m := (pack_semiring T _ id_phant _ id_phant m).

This semiring packager notation SemiringType T m can be read as: “find bT of type Monoid.type such that T unifies with Monoid.sort bT, find b of type Monoid.class_of T such that b unifies with Monoid.class bT, and build a semiring instance Semiring.Pack T (Semiring.Class T b m)”. The first occurrence of the [find ...] notation in pack_semiring hides two binders
fun (bT : Monoid.type) (_ : phantom T → phantom (Monoid.sort bT)) ⇒ ...

where phantom is defined as follows:
Variant phantom {T : Type} (p : T) : Prop := Phantom : phantom p.

The SemiringType notation instantiates the above binders with two arguments
_ id_phant where id_phant is an identity function of type phantom t →
phantom t (for some t), so that T unifies with Monoid.sort bT to instantiates bT with the canonical monoid instance for T. The second occurrence of the [find ...] notation coerces Monoid.class bT of type Monoid.class_of bT to type
Monoid.class_of T by unification.

The canonical semiring instance for Z can be redefined by using the semiring packager as follows.

Canonical Z_semiringType := SemiringType Z Z_semiring.

Notably, if we declare the monoid instance Z_monoidType as Definition instead of Canonical, type-checking the above declaration Z_semiringType fails with the message
'Error: Z "is not an Monoid.type"

so that the user can find a fact that the canonical monoid instance for Z has not been declared yet.

As a side note, if one omits the type argument of a packager with a placeholder as follows, the packager may behave unpredictably as a unification hint as we mentioned in Sect. 7.

Canonical bad_Z_semiringType := SemiringType _ Z_semiring.

The placeholder in the above declaration is instantiated with Monoid.type
Z_monoidType by the first occurrence of [find ...] notation in pack_semiring; thus, a unification hint that overwrites the join of semiring and monoids with the concrete type Z will be synthesized, and the assertion for that join
check_join Semiring.type Monoid.type Semiring.type.

fails with the following message:
The join of Semiring.type and Monoid.type is a concrete type Z but is expected to be Semiring.type.

The group packager and the canonical group instance for Z can similarly be (re)defined as follows.
**Definition** pack_group (T : Type) :=
[find bT : Monoid.type | T ∼ Monoid.sort bT | "is not an Monoid.type"
][find b : Monoid.class_of T | b ∼ Monoid.class bT ]
fun m : Group.mixin_of (Monoid.Pack T b) =>
Group.Pack T (Group.Class T b m).

**Notation** GroupType T m := (pack_group T _ id_phant _ id_phant m).

**Canonical** Z_groupType := GroupType Z Z_group.

Since the ring structure inherits from groups and semirings and has no further axiom, the ring packager can be defined as the following notation that only takes a type; internally, it finds the canonical group and semiring instances for the given type and construct a ring instance from them.

**Definition** pack_ring (T : Type) :=
[find gT : Group.type | T ∼ Group.sort gT | "is not an Group.type"
][find g : Group.class_of T | g ∼ Group.class gT ]
[find sT : Semiring.type | T ∼ Semiring.sort sT | "is not an Semiring.type"
][find s : Semiring.mixin_of (Monoid.Pack T (Group.base T g)) | s ∼ Semiring.mixin _ (Semiring.class sT )]
Ring.Pack T (Ring.Class T g s).

**Notation** RingType T := (pack_ring T _ id_phant _ id_phant _ id_phant _ id_phant).

**Canonical** Z_ringType := RingType Z.

In the above definitions, each packager notation of a structure takes canonical instances of its (direct) superclasses for a given type, and constructs an instance of the structure using mixins and classes included in that canonical instances; thus, they enforce Proposition B.1 on canonical instances, which can be confirmed by the following Ltac script.

unify (Semiring.monoidType Z_semiringType) Z_monoidType.
unify (Group.monoidType Z_groupType) Z_monoidType.
unify (Ring.monoidType Z_ringType) Z_monoidType.
unify (Ring.semiringType Z_ringType) Z_semiringType.
unify (Ring.groupType Z_ringType) Z_groupType.

In general, if packagers are defined and used properly, Proposition B.1 should hold. Users can still bypass the packager mechanism and construct canonical instances that do not respect the invariant, but practically packagers work to enforce the invariant.

### C  Omitted lemmas and proofs for Sect. 5

This appendix shows informal statements and proofs of lemmas that prove Theorem 5.1 and the complete formalization of Sect. 5 in Coq. For each part, informal ones come before formal ones.

**From** mathcomp Require Import ssreflect ssrfun ssrbool eqtype ssrnat seq choice.
**From** mathcomp Require Import fintype order finset.

**Set Implicit Arguments.**
**Unset Strict Implicit.**
Validating Mathematical Structures

Lemma C.1. The strict inheritance relation $\Rightarrow^+$ and its inverse relation $\Leftarrow^+$ are well-founded relations.

Proof. Strict partial orders on a finite set are well-founded. □

Lemma finlt_wf disp (T : finPOrderType disp) : well_founded (<%O : rel T)%O.
Proof. move⇒ x.
have: |< x|%O ≤ |T| by exact: max_card.
elim: |T| x ⇒ [\n ihn x hx; constructor ⇒ y hy.
- have: y ∈ enum (< x)%O by rewrite mem_enum.
  by move: hx; rewrite cardE /=; case: (enum _).
- apply: ihn; rewrite ltnS; apply/(ltn_trans _ hx)/proper_card.
  apply/properP; split.
  + by apply/subsetP ⇒ ?; move/lt_trans; apply.
  + by exists y ⇒ //; rewrite inE ltxx.
Qed.

Lemma fingt_wf disp (T : finPOrderType disp) : well_founded (>%O : rel T)%O.
Proof. exact: (@finlt_wf _ [finPOrderType of Order.converse T]). Qed.

Let us assume S is the type of structures whose ordering is the inheritance relation: $a \leq b$ and $a < b$ mean b non-strictly and strictly inherits from a respectively.

Section join_structures_meta_properties.
Variables (disp : unit) (S : finPOrderType disp).

Definition 5.2 is as follows.

(* Weak and strict subclasses. *)
Definition w_subclasses (b : S) : {set S} := [set a | b \leq a]%O.
Definition s_subclasses (b : S) : {set S} := [set a | b < a]%O.

(* Minimal common subclasses. *)
Definition mcs (a b : S) : {set S} :=
  let subs := w_subclasses a :&: w_subclasses b in
  subs \b: \bigcup_(c in subs) s_subclasses c.

Definition 5.3 is as follows.

(* For any structure ‘a’ and ‘b’, their join must be unique. *)
Hypothesis (unique_join : \forall a b : S, |mcs a b| \leq 1).

Definition 5.4 is as follows.

(* The type of structures extended with the top (undefined) structure. *)
Definition extS := option S.

(* Ordering of ‘S’ can be naturally extended to ‘extS’ as follows. *)
Definition le_extS (a b : extS) : bool :=
  match b, a with
Definition `lt_extS (a b : extS) : bool :=
  match a, b with
  | None, None ⇒ false
  | Some _, None ⇒ true
  | None, Some _ ⇒ false
  | Some a, Some b ⇒ a < b
end%O.

Lemma C.2. An extended hierarchy Ⅎ is (non-strictly) partially ordered by its inheritance relation Ⅎ∗.

Proof. The reflexivity, antisymmetry and transitivity of Ⅎ∗ should be checked here. The proofs are by case analysis.

Lemma `lt_extS_def a b : lt_extS a b = (b \neq a) && le_extS a b.
Proof. by case: a b ⇒ [a|][b|] \neq; rewrite lt_def. Qed.

Lemma le_extS_refl : reflexive le_extS. Proof. by case⇒ /=. Qed.

Lemma le_extS_anti : antisymmetric le_extS.
Proof. by case⇒ [a|][b|] // /le_anti. Qed.

Lemma le_extS_trans : transitive le_extS.
Proof. by case⇒ [?][?][?] //; exact: le_trans. Qed.

Definition extS_porderMixin :=
  LePOrderMixin lt_extS_def le_extS_refl le_extS_anti le_extS_trans.
Canonical extS_porderType := POrderType disp extS extS_porderMixin.

Lemma le_extS_SomeE a b : (Some a \leq Some b :> extS)%O = (a \leq b)%O.
Proof. by []. Qed.

Lemma lt_extS_SomeE a b : (Some a < Some b :> extS)%O = (a < b)%O.
Proof. by []. Qed.

Definition 5.5 is as follows.
Definition join (a b : extS) : extS :=
  match a, b with
  | Some a, Some b ⇒
      if enum (mcs a b) is c :: _ then Some c else None
  | _, _ ⇒ None
  end.

Lemma C.3. For an extended hierarchy, ⊤ is the absorbing element.

Proof. By definition.

Lemma joinNx : left_zero None join. Proof. done. Qed.
Lemma joinxN : right_zero None join. Proof. by case. Qed.
Lemma C.4. For an extended hierarchy, the join is idempotent:

\[
\forall A \in \mathcal{H}, \text{join}(A, A) = A.
\]

Proof. If \( A = \top \), \( \text{join}(A, A) = A \) is true by Definition 5.5; otherwise, it is sufficient to show \( \text{mcs}(A, A) = \{A\} \). Let us prove they are extensionally equal.

\[
B \in \text{mcs}(A, A) \\
\Leftrightarrow A \Rightarrow^* B \land \neg(\exists A' \in \mathcal{H}, A \Rightarrow^* A' \land A' \Rightarrow^+ B) \quad \text{(Definition 5.2)}
\]

If \( A \Rightarrow^* B \) does not hold, the above formula is false; also, the RHS \( B \in \{A\} \) (\( \Leftrightarrow A \Rightarrow^* B \land B \Rightarrow^* A \)) is false. Thus, let us consider the case \( A \Rightarrow^* B \) holds.

\[
\Leftrightarrow \neg(\exists A' \in \mathcal{H}, A \Rightarrow^* A' \land A' \Rightarrow^+ B) \\
\Leftrightarrow \neg(A \Rightarrow^+ B) \quad \text{(Transitivity)}
\]

\[
\Leftrightarrow \neg(A \neq B) \quad \text{(Assumption)}
\]

\[
\Leftrightarrow B \in \{A\}
\]

The above transformation shows \( \text{mcs}(A, A) = \{A\} \); thus, the join is idempotent. 

\[\square\]

Lemma joinxx: idempotent join.

Proof. case \( \Rightarrow [a|] /=; \) rewrite /mcs setIid; set \( A := _ : _ : _ \).

suff \( \Rightarrow \): \( A = [\text{set } a] \) by rewrite enum_set1.

rewrite \{}\text{}/A; apply/setP \( \Rightarrow b \).

rewrite !\text{inE eq_le andbC} \text{[RHS andbC]; case: (boolP (a \leq b) \text{[O]} \Rightarrow /= \text{Hab}.}

apply/bigcupP; case: ifP \( \Rightarrow [Hba [c]| Hba] \).

- by rewrite !\text{inE} \Rightarrow \text{Hac}; move/(le_lt_trans (le_trans Hba Hac)); rewrite ltxx.

- by exists a; rewrite !\text{inE} //; rewrite lt_def Hab andbT eq_le Hba.

Qed.

Lemma C.5. For an extended hierarchy, the join is commutative:

\[
\forall A, B \in \mathcal{H}, \text{join}(A, B) = \text{join}(B, A).
\]

Proof. Since the join is defined symmetrically with respect to the parameters in Definitions 5.2 and 5.5, it is commutative. \[\square\]

Lemma joinC: commutative join.

Proof. by move\( \Rightarrow [a][b] /=; \) rewrite /mcs setIC. Qed.

Lemma C.6. For any structures \( A \) and \( B \) in an extended hierarchy \( \mathcal{H} \), \( \text{join}(A, B) \) non-strictly inherits from both \( A \) and \( B \):

\[
A \Rightarrow^* \text{join}(A, B), \quad B \Rightarrow^* \text{join}(A, B).
\]

Proof. If \( A = \top, B = \top \), or \( \text{mcs}(A, B) \) is not a singleton set, \( \text{join}(A, B) = \top \) holds; thus, it inherits from both \( A \) and \( B \). Otherwise, \( \text{mcs}(A, B) \) is a singleton set \( \{C\} \) and \( \text{join}(A, B) = C \) holds. \( C \) inherits from both \( A \) and \( B \) by Definition 5.2. \[\square\]
Lemma join_inherit_l a b : (a ≤ join a b)%O.
Proof.  
case: a b ⇒ [a|][b|] //=.
suff: ∀ c, c ∈ enum (mcs a b) → (a ≤ c)%O 
  by case: (enum _) ⇒ // c ? /(_ c); rewrite inE eqxx /=; exact.
by move ⇒ c; rewrite mem_enum; case/setDP ⇒ /=; rewrite inE.
Qed.

Lemma join_inherit_r a b : (b ≤ join a b)%O.
Proof. by rewrite joinC join_inherit_l. Qed.

Lemma C.7. For any structures A, B, and C in an extended well-formed hierarchy \( \mathcal{H} \), C non-strictly inherits from join(A, B) if and only if C non-strictly inherits from both A and B:

\[ \text{join}(A, B) \rightsquigarrow^{+} C \iff A \rightsquigarrow^{+} C \land B \rightsquigarrow^{+} C. \]

Proof. If A, B, or C is \( \top \), this proposition is trivial by Definitions 5.4 and 5.5; also, the direct implication is trivial by Lemma C.6 and the transitivity of \( \rightsquigarrow^{+} \). Thus it is sufficient to prove the converse implication for \( A, B, C \in \mathcal{H} \). Let us name \( C \) the common subclasses of \( A \) and \( B \), which is \( \{C \in \mathcal{H} | A \rightsquigarrow^{+} C \land B \rightsquigarrow^{+} C\} \), and prove the following proposition by well-founded induction on \( C \in \mathcal{H} \):

\[ C \in C \Rightarrow \text{join}(A, B) \rightsquigarrow^{+} C. \]

If mcs(\( A, B \)) is empty, \( C \) is a subset of \( \{C \in \mathcal{H} | \exists C' \in C, C' \rightsquigarrow^{+} C\} \) by Definition 5.2; thus, \( C' \rightsquigarrow^{+} C \) holds for some \( C' \in C \) by the assumption \( C \in C \). By the induction hypothesis on \( C' \), join(A, B) \( \rightsquigarrow^{+} C' \ (\rightsquigarrow^{+} C) \) holds.

If mcs(\( A, B \)) is not empty, it is a singleton set \( \{\text{join}(A, B)\} \) because of the uniqueness of join; then, the following equation holds by Definition 5.2:

\[ C = \{\text{join}(A, B)\} \cup \{C \in \mathcal{H} | \exists C' \in C, C' \rightsquigarrow^{+} C\}. \]

By the assumption, \( C \) inhabits \( \{\text{join}(A, B)\} \) or \( \{C \in \mathcal{H} | \exists C' \in C, C' \rightsquigarrow^{+} C\} \). If \( C = \text{join}(A, B) \), the conclusion is true by reflexivity; otherwise, \( C' \rightsquigarrow^{+} C \) holds for some \( C' \in C \). By the induction hypothesis on \( C' \), join(A, B) \( \rightsquigarrow^{+} C' \ (\rightsquigarrow^{+} C) \) holds.

Lemma le_joinE a b c : (join a b ≤ c)%O = (a ≤ c)%O && (b ≤ c)%O.
Proof.  
apply/idP/idP ⇒ [le_ab c|/andP []].
rewrite (le_trans (join_inherit_l _ _) le_ab_c).
exact: (le_trans (join_inherit_r _ _) le_ab_c).
case: a b c ⇒ [a|][b|][c|] //; rewrite !le_extS_SomeE ⇒ le_ac le_bc.
set sub_ab := w_subclasses a :&: w_subclasses b.
have {le_ac le_bc}: c ∈ sub_ab by rewrite inE; apply/andP; split.
elim/Acc_ind: c / (finlt_wf c) ⇒ c _ ihc hc.
move: (unique_join a b); rewrite leq_eqVlt ltnS leqn0 cards_eq0 setD_eq0.
case/orP ⇒ ![cardsIP [join_ab joinsE] | hsub]; last first.
case/(subsetP hsub)/bigcupP: (hc) ⇒ y hy; rewrite inE ⇒ lt_yx.
exact/(le_trans (ihc _ lt_yx hy))/ltW/lt_yx.
move: ihc hc; rewrite /join joinsE enum_set1 le_extS_SomeE ⇒ ihc.
suff →: sub_ab = join_ab \: \bigcup (c in sub_ab) s_subclasses c.
Lemma C.8. For an extended well-formed hierarchy, the join is associative:

$$\forall A B C \in \mathcal{H}, \text{join}(\text{join}(A, B), C) = \text{join}(A, \text{join}(B, C)).$$

Proof. The above equation has the following equivalent formula:

$$\text{join}(\text{join}(A, B), C) = \text{join}(A, \text{join}(B, C)) \iff \text{join}(\text{join}(A, B), C) \bowtie^* \text{join}(A, \text{join}(B, C)) \land \text{join}(A, \text{join}(B, C)) \bowtie^* \text{join}(A, B, C)$$

(antisymmetry and reflexivity of $\bowtie^*$)

$$\iff A \bowtie^* \text{join}(A, \text{join}(B, C)) \land B \bowtie^* \text{join}(A, \text{join}(B, C)) \land C \bowtie^* \text{join}(A, \text{join}(B, C)) \land A \bowtie^* \text{join}(A, B, C) \land B \bowtie^* \text{join}(A, B, C) \land C \bowtie^* \text{join}(A, B, C)$$

(Lemma C.7).

Each clause of the above formula is a corollary of Lemma C.6. □

Lemma joinA : associative join.
Proof.
move⇒ a b c; apply/eqP; rewrite (eq_le _ (join _ _));
  apply/andP; split; rewrite !le_joinE -?andbA; apply/and3P; split.
- exact/(le_trans (join_inherit_l _ _))/join_inherit_l.
- exact/(le_trans (join_inherit_r _ _))/join_inherit_l.
- exact: join_inherit_r.
- exact: join_inherit_l.
- exact/(le_trans (join_inherit_l _ _))/join_inherit_r.
- exact/(le_trans (join_inherit_r _ _))/join_inherit_r.
Qed.

Theorem 5.1 consists of Lemmas C.4, C.5, and C.8; thus holds.
End join_structures_meta_properties.

D Evolution of the hierarchy in Mathematical Components

In this appendix, we report in detail recent efforts on fixing and extending the hierarchy of structures in the Mathematical Components library. In those improvements, our tools help us and other contributors to Mathematical Components to find inheritance bugs, moreover, improve the development process by reducing the reviewing and maintenance burden, and allow developers and contributors to focus on mathematical contents and other design issues.
D.1 Mathematical Components 1.7.0

We start with the hierarchy of Mathematical Components 1.7.0 which is depicted in Fig. 4, lacks 7 inheritance edges from the CountRing structures to the FinRing structures, and contains some other inheritance bugs. Those missing edges do not mean just missing inference rules, but also breaks the well-formedness invariant. For instance, countType and zmodType have two ambiguous joins countZmodType and finZmodType due to the missing edge from the former one to the latter one. The same issues can be seen in the ringType, comRingType, unitRingType, comUnitRingType, idomainType, and fieldType structures, and their corresponding countable and finite structures. There are also the following 8 missing canonical projections:

- the join of countClosedFieldType and countIdomainType which should be countClosedFieldType,
- the join of countType and lmodType which should be finLmodType,
- the join of countType and lalgType which should be finLalgType,
- the join of countType and algType which should be finAlgType,
- the join of countType and unitAlgType which should be finUnitAlgType,
- the join of finUnitRingType and unitAlgType which should be finUnitAlgType,
- the join of fieldType and numDomainType which should be numFieldType, and
- the join of fieldType and realDomainType which should be realFieldType.
Fig. 5. The hierarchy of structures in the Mathematical Components library 1.8.0 and 1.9.0. The bold dashed edges highlight new inheritance edges that are missing in 1.7.0.

The join of finType and countType should be finType, but has been overwritten by the canonical finType instance for extremal_group as explained in Sect. 7.

D.2 Mathematical Components 1.8.0 and 1.9.0

All the above inheritance issues in Mathematical Components 1.7.0 have been addressed in version 1.8.0 whose hierarchy of structures is depicted in Fig. 5. In this diagram, the bold dashed edges highlight new inheritance edges that are missing in 1.7.0. Any implementation of structures and their inheritance has not been changed in Mathematical Components 1.9.0 from version 1.8.0. Cohen [11] made the initial attempt to add missing inheritances from CountRing to FinRing structures without any tooling work; however, this attempt was incomplete. Then we made the second attempt to fix them with prior tooling work of Sect. 6 by Cohen [37], which check only the existence of canonical projections but do not check which structure is inferred. In this change, we added all the missing canonical projections thanks to the tool, but did not fix the canonical finType instance for extremal_group and also introduced a few misplaced canonical projections, because of the incompleteness of the checking. Finally we made the initial complete implementation of the well-formedness checking [13] as in Sect. 6, and fixed all the inheritance issues we discovered.
D.3 Mathematical Components 1.10.0

In Mathematical Components 1.10.0, Hivert [24] added new structures comAlgType and comUnitAlgType, which are interfaces for non-unitary and unitary commutative algebras respectively. The hierarchy of this version is depicted in Fig. 6, where the new structures and inheritance edges added are highlighted by bold frames and bold dashed edges respectively. This extension requires to change the field extension (fieldExtType) and splitting field (splittingFieldType) structures to inherit from those commutative algebra structures, which involves some additions and deletions of joins; for instance, each join of lmodType, lalgType, algType, unitAlgType, and comRingType, comUnitRingType is fieldExtType in 1.9.0, but should be generalized to one of the new commutative algebra structures. In this extension process, they fixed some inheritance issues with help from us and our well-formedness checking tool; at the same time, we made sure there is no inheritance bug without reviewing the whole boilerplate code of implicit coercions and canonical projections.

D.4 The current master branch of Mathematical Components

In the current master branch of Mathematical Components which supposed to be released as a part of version 1.11.0, we ported the order sub-library of the mathcomp-finmap library [12] to Mathematical Components [14]. The hierarchy of this version is depicted in Fig. 7, where the new structures and inheritance edges
Fig. 7. The hierarchy of structures in the Mathematical Components library (the master branch of the GitHub repository on Dec. 30, 2019, the commit hash is: a93a392121e8e02c6fdaa6c674dd90af8b12c28d). New structures and inheritance edges are highlighted by bold frames and bold dashed edges respectively.

added are highlighted by bold frames and bold dashed edges respectively. The order sub-library provides several structures of ordered types, including partially ordered types \texttt{porderType}, distributive lattices \texttt{distrLatticeType}, and totally ordered types \texttt{orderType}; thus, this extension requires to change the ordered domain and ordered field structures (\texttt{numDomainType} and its subclasses) to inherit from those ordered type structures. We also factored out normed Abelian groups from the partially ordered domain structure \texttt{numDomainType} as a new structure \texttt{normedZmodType}, to unify several notions of norms in the Mathematical Components Analysis library. This refactoring work became approximately 10,000 lines of changes; thus, reducing the reviewing burden was an even more critical issue.