Multi-Model Probabilistic Programming

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Abstract

Probabilistic programming makes it easy to represent a probabilistic model as a program. Building an individual model, however, is only one step of probabilistic modeling. The broader challenge of probabilistic modeling is in understanding and navigating spaces of alternative models. There is currently no good way to represent these spaces of alternative models, despite their central role.

We present an extension of probabilistic programming that lets each program represent a network of interrelated probabilistic models. We give a formal semantics for these multi-model probabilistic programs, a collection of efficient algorithms for network-of-model operations, and an example implementation built on top of the popular probabilistic programming language Stan.

This network-of-models representation opens many doors, including search and automation in model-space, tracking and communication of model development, and explicit modeler degrees of freedom to mitigate issues like p-hacking. We demonstrate automatic model search and model development tracking using our Stan implementation, and we propose many more possible applications.
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1 Introduction

A probabilistic program is a program that represents a probabilistic model. Probabilistic programming suggests an analogy between software engineering and probabilistic modeling: developing a model is like developing a program. However, there is a key difference: while there are only ever a handful of relevant versions of a program in development, there are often a multitude of alternative probabilistic models that remain relevant throughout development, communication and validation. Probabilistic programming systems currently ignore this multiplicity.

We present an extension of probabilistic programming that lets users encode networks of models, graphs of models connected by similarity. Just as probabilistic programs let users represent and query probabilistic models, these multi-model probabilistic programs let users represent and query networks of probabilistic models.

1.1 Uses of networks of models

We focus on four categories of use cases for networks of probabilistic models:

1. Automation in model-space

Networks of models allow us to deploy automation in model-space. For example, algorithms can search for models or neighborhoods in the network that optimize a real-valued model scoring function. We demonstrate a greedy graph search in section 9.3 and more advanced search methods are discussed in section 10. Other examples of automation on networks include:

- **Stacking** methods seek an optimal weighted subset of the models to combine into a high-performing ensemble or “stacked” model [1].
- **Projection prediction** methods search for the “simplest” model that reproduces the predictions of a gold standard model or ensemble [2].

2. Understanding the problem and its solution space.

Statisticians often use multiple related models to gain insight into their problem and solution space [3]. Examples include:

- Plotting alternative models by evaluation metrics to understand trade-offs such as model complexity vs. accuracy [4].
• Comparing diagnostic samples, such as posterior predictive samples, to understand the impact of model decisions [5].
• Applying “multiverse” methods, which seek to quantify modeling uncertainty by sampling from a whole set of plausible models [6].

3. Tracking and communicating the branching path of development.

Probabilistic model development is an inherently iterative and branching process: models are improved by a cycle of criticism and adjustment [3, 7]. Development follows an often-backtracking path through model space; a path that model developers often have difficulty managing [8, 9, 10].

When the relevant region of model space is explicitly represented as a network of models, the path of development can also be explicitly documented. This documentation is useful for managing development [10], for third parties interested in learning from or extending the work, and, as discussed in case 4, as context for third-party auditors assessing the quality of the final model.

Standard version control tools like Git can serve this use case to some extent, but as the case study in section 9.2 shows, the network of models abstraction earns more than version control: it keeps all relevant models available and tracks their semantic relationships. Two surveys of data scientists, one by Guo and one by Kery et al., both report that version control is not typically used for managing exploratory data analysis [8, 10].

4. Making modeler degrees of freedom explicit.

P-hacking [11] and the Garden of Forking Paths [12] are issues in statistics with a common root cause called modeler degrees of freedom [13]: when a modeling task, such as the analysis of scientific data, includes modeling decisions with multiple justifiable solutions, the modeler can, intentionally or not, tune their solutions to cherry-pick a desirable model, such as a model with a “significant” p-value.

There are two ways in which explicit networks of models can alleviate the issues of modeler degrees of freedom. The first way is to aid in reporting the set of analyses that were done. Wigboldus and Dotsch, discussing questionable research practices, argue: “the potentially (highly) questionable part of your actions as a researcher is not
that you engage in all kinds of exploratory analyses. Instead, the ques-
tionable part is not reporting truthfully and explicitly the exploratory
nature of these analyses” [14]. When researchers explicitly report their
path of exploration through the network of models, their degrees of
freedom become transparent.

The second way is to automate sensitivity analysis. Sensitivity analy-
ses aim to “assess whether altering any of the assumptions made leads
to different final interpretations or conclusions” [15]. They are broadly
recommended for scientific reports such as clinical trials [16]. In a
survey of solutions to researcher degrees of freedom, Rubin finds that
sensitivity analyses “provide an effective solution to the p-hacking prob-
lem”, and also the Forking Paths problem in some cases [17]. Explicit
networks of models let both researchers and third-party auditors au-
tomate sensitivity analysis by a simple procedure: for each conclusion
drawn from a final model, check the extent to which that conclusion is
also drawn by the model’s neighbors. When each neighbor differs by
one modeling decision, the analysis tells us the modeling decisions on
which the conclusions depend.

Some of these use cases, like automated model search and visualizations
of model space, are achieved in practice only by those with sufficient time and
expertise to implement ad-hoc methods with hand-enumerated sets of mod-
els. Other use cases, like explicit modeler degrees of freedom and automated
sensitivity analysis, are rarely ever achieved in practice despite being val-
uable in theory. We argue that all of these use cases could become convenient
and routine if we had a standard representation of networks of models.

We note that each of the four use cases above has a natural definition
and utility for drawing edges between models:

- For use case 1 (automation), edges should be between the most similar
  models: the network is then more analogous to a continuous and dif-
  ferentiable space, and methods like greedy graph search more closely
  approximate gradient descent.

- For use case 2 (solution space mapping), again edges should be between
  the most semantically similar models; edges then provide a more con-
  sistent sense of distance and orientation.

Rubin distinguishes between result-biased and result-neutral Forking Paths, and finds
that sensitivity analysis is not necessarily sufficient for result-neutral cases.
• For use case 3 (tracking and communicating development), edges should bridge sequential versions of a model. Authors and auditors then can cleanly trace model development, with each of its decision points and model transformations, as a tree within the network.

• For use case 4 (explicit degrees of freedom), edges should be between model pairs that are that are one “decision” apart; then each edge is like a step in the Garden of Forking Paths.

Ideally, a standard construction of model networks should be compatible with all of these use cases.

### 1.2 Representing networks of models

To support all of the above use cases, representations of networks of models should support the following operations efficiently:

1. **Explicitly generate the network of models (if practical).**

2. **Given a node, generate its set of neighbors.** This operation becomes necessary when the network is too large to practically generate in its entirety; for instance, when we are searching through a large model space.

3. **Given a node, generate its corresponding probabilistic program.**

In addition, we would like our representation to be:

1. **Easy to read and understand.** Especially for cases 3 and 4, clarity is the priority.

2. **Simple to write.** Probabilistic modelers may not be expert programmers.

3. **Scalable to many models.** If a representation is too redundant, large numbers of models become cumbersome.

4. **Standardized.**

   A standard format enables a stable network-of-models API to easily build general model-space tools.
One obvious choice for representing multiple models is a directory of relevant probabilistic programs. According to surveys done by Guo and Kery et al., this is the typical solution among data scientists [8, 10].

While appealing for their simplicity, file collections are a poor solution because they become uninterruptible, unmanageable, and memory intensive as the number of models grows large, and because they discard the semantic relationships between models. Kery et al. also report that data scientists have issues with file naming, keeping track of the relationships between files, and maintaining a mental map of their code [10].

Another possible choice of representation is a program in a general-purpose language that generates the set of probabilistic programs. This approach is flexible and scalable, but its flexibility also makes it prohibitively difficult to write, understand, and standardize.

Our proposed representation is a middle ground: a meta-programming feature to augment existing probabilistic programming languages, so that meta-programs, which we call multi-model programs, represent networks of probabilistic models. We argue that our meta-programming approach is nearly as flexible as general program generation and easier to write and understand than the directory-of-programs approach for nontrivial examples. We call our meta-programming feature swappable modules.

1.3 Swappable modules in Stan

To demonstrate swappable modules, we use Stan as our example host language, mainly because Stan is popular, performant, and has a clear, established semantics [18, 19]. Stan is also a highly structured and restrictive language, so by adding a swappable modules to Stan, we are demonstrating an usually difficult case that can easily be transferred to other languages.

We refer to the Stan language augmented with swappable modules as modular Stan. We have built a prototype compiler [20] and interactive visualization website [21] for modular Stan.

Figure 1 shows an abstracted modular Stan program and two data structures derived from it.

A modular Stan program is made of two parts. The first part is the base. The base is like a Stan program, except that its code can contain holes, which are syntactically similar to function calls but are more flexible. The second part is a list of module implementations. Each module implementation describes a new way to “fill” a particular hole. More than one module implementation be specified to “fill” the same hole. Module implementations can themselves contain holes.
Figure 1: The correspondence between a modular Stan program and a network of models. Holes are represented as empty shapes. Modules are represented as filled shapes, with the same shape as the hole that they fill and a unique color. (a) and (b) represent a modular Stan program in its two parts, the base (a) and the module implementations (b). (c) represents the relationships between the base, holes and modules implementations. (d) represents the model graph, where each node is a model corresponding to a valid selection of modules, and each edge is labeled with the hole by which its endpoints differ. (e) shows the Stan program corresponding to a node; it is synthesized from the selected modules of the node.
We can visualize the holes and implementations, with their implementation-fills-hole and code-contains-hole relationships, as a rooted directed acyclic graph of base, hole and module implementation nodes, where the root represents the program’s base, each base and module implementation node points to the holes it contains, and each hole node points to the module implementations that fill it. We refer to this graph as the module graph of a program. The module graph is not necessarily a tree because multiple pieces of code can contain the same hole.

To build a valid Stan program out of a modular Stan program, we need to select one module implementation to fill each hole in its base, and one implementation to fill each hole in those implementations, and so on, until there are no holes. A minimal set of module implementations that leaves no empty holes is called a valid selection. Given a modular Stan program and a valid selection, we can produce a valid Stan program by filling each hole with the given module implementation.

A modular Stan program can therefore represent many Stan programs: one for each valid selection. If we consider each of these Stan programs to be a node, we find a natural network structure: draw an edge between two Stan program nodes when their selections conflict by only one choice. Figure 1 shows such a graph with correspondence of each single node to a Stan program and thereby to a probabilistic model. We argue that this graph construction is a powerful way to represent networks of models.

Holes and module implementations are like function calls and function definitions, but with important differences:

- Selecting a module implementation can add model parameters and have other changes that are not local to their call site. Stan requires the set of parameters to be fixed at compile time; therefore modules are selected before Stan’s compile time.

- More than one module implementation can be specified to fill a hole, like function overloading but with identical type signatures.

- Because module implementation code is essentially inlined statically, holes can appear in places where function calls cannot.

By defining a module system for Stan, we are also incidentally letting users write their normal Stan programs in a more modular way. Modularity of this level is a feature that is both important for probabilistic modeling workflow [3] and conspicuously absent from probabilistic programming languages like Stan [22].
Probabilistic programming languages augmented with swappable modules meet all of our earlier criteria to represent networks of models:

- They are easy to read and write, because only one abstraction (the `module`) and a small amount of syntax is introduced on top of the host language, and the `module` abstraction already fits naturally into the probabilistic modeling workflow [3].

- They are scalable, because the combinatory nature of implementation selection can define many models with little code. The language extensions in section 7 further increase that expressiveness.

- They are standardized, because compilers enforce well-defined languages.

- The required network-building, neighbor-finding and model-selection operations can be implemented efficiently.

In addition, the definition of edges as between models that differ by one choice module is compatible with all four uses cases’ definitions of edges.

In this paper we introduce the syntax, semantics, and operation algorithms of a swappable module system for Stan. For each algorithm we provide proofs of completeness, correctness and efficiency.

We also introduce language extensions and macros to conveniently express common patterns of model variation in terms of our module system. We also introduce a macro system to concisely express common patterns of model variation and large, complex model families.

We demonstrate some of the benefits of multi-model probabilistic programs with two brief but real-world data science case studies.

2 Related work

The 'network of models' is an established concept in statistics and machine learning, but explicit and general network of models abstractions are not supported within probabilistic programming languages or other statistical software. For instance, multi-model methods like ensemble methods and model search are common in machine learning, but are typically ad-hoc in that they do not start with a declarative network topology for their set of model. The closest method that we are aware of is perhaps grid search, which searches a pre-defined grid of model hyperparameters.
There are existing probabilistic programming systems which allow users to define their programs by combining probabilistic subcomponents. For example, Prophet [23] allows users to combine subcomponents into time-series models. This effect could also be achieved in embedded probabilistic programming languages whose host languages have sufficiently expressive module systems. We are not aware of any other module systems specialized to encapsulate flexible components of structured probabilistic programs.

Kery et al. developed a tool for code editors, Variolite, to support exploratory data science by tracking alternative snippets of code in version control. Variolite lets developers write, visualize and manage iterative and branching versions of data science pipelines in a similar way to our proposal. Variolite addresses what we call use case 3 (development tracking). Variolite differs from our system primarily in that it is a tool for code editors rather than a metaprogramming feature, it does not produce a network of models, and because it is language agnostic, it only supports swapping out regions of code rather than more general semantic units.

There are existing systems that allow users to specify a program’s components at compile-time. Backpack [24] is a build-system tool for the Haskell ecosystem that lets users swap out external software libraries that implement a common interface. Much of work done by Yang to introduce Backpack as a mixin linker also applies to our swappable module system. In practice, the C preprocessor is often used for this purpose; it can include or exclude sections of code depending on user flags or system environment properties. These systems are not commonly applied to probabilistic programs or to study networks of programs.

2.1 Comparison to ML-like module systems

Our swappable module system bears some resemblance to ML-like module systems [25, 26]. We find OCaml to be a helpful comparison point [27]. The hole and module approach can be understood in the language of ML-like modules:

Each hole in a program, which is to say each unique hole identifier referenced in a program, can be thought of as declaring a module signature and a module-valued variable of that signature. Each statement and expression referencing a hole is like a reference to a field of that hole’s corresponding variable. A hole’s variable may take the value of any module that “implements” it. A hole’s signature is inferred from its usage and implementations. The value assigned to a hole’s variable may either be specified outside of the program or left non-deterministic. Blocks of code that contain holes
can then be thought of as ML functors in that their holes are like implicit module-valued arguments.

However, unlike ML-like modules:

1. Modules are not applied at any point in the program. Rather, the programs’ semantic domain is the set of programs generated by any combination of module applications, as though module applications were non-deterministic; then the user can determine the modules to apply in an optional mode of compilation called concretization that we discuss in section 6.1.

2. When a module is assigned to a hole, or selected, there can be global effects on the semantics of the program, because the module may add code to Stan’s top-level blocks. For instance, a module may introduce a new model parameter, which changes the domain over which the program defines a joint distribution. This effect is especially noteworthy in languages like Stan in which model parameters are fixed at compile time, because it implies that module application must happen before compile time.

We are not aware of prior examples of inferred implicit module signatures, non-deterministic functor application semantics, or module application with non-local effects on the resulting program.

3 Background: Stan

Stan is our example host language, so we give a brief overview of Stan programs and of Stan’s syntax in this section.

Like all probabilistic programs, Stan programs represent probabilistic models. Stan programs are C-like, imperative, and are written as a sequence of top-level blocks. Here is a simple example of a Stan program:

```stan
data {
  int N;
  vector[N] x;
}
parameters {
  real mu;
  real sigma;
}
model {
```
mu ~ normal(0, 1);
sigma ~ lognormal(0, 1);
x ~ normal(mu, sigma);

We see three of Stan’s blocks: data, parameters, and model. The data block declares the observed variables and the parameters block declares the unobserved variables. The model block define the log-density of the joint distribution of the observed and unobserved variables. Each ~ statement implicitly increments a variable target that represents the value of the overall log-density function; for instance, mu ~ normal(0, 1); could be rewritten target += normal_lpdf(mu, 0, 1).

The above program represents the probabilistic model:

\[
\begin{align*}
\mu & \sim \text{Normal}(0, 1) \\
\sigma & \sim \text{LogNormal}(0, 1) \\
x & \sim \text{Normal}(\mu, \sigma)
\end{align*}
\]

where \(x\) is an observed variable. When the program is compiled and executed given data for \(x\), it should produce samples from the posterior distributions \(P(\mu | x)\) and \(P(\sigma | x)\).

For our purposes, it is sufficiently precise to take the semantic domain of a Stan program \(p\), \([p]\), to be a joint distribution \(P(d, \theta)\) of the variables declared in the data block, \(d\), and parameters block, \(\theta\), of \(p\), from which can be inferred a posterior distribution \(P(\theta | d)\).

### 3.1 Syntax

Stan programs are organized into blocks of statements that describe different aspects of a probabilistic model. Each is an ordered subset of blocks:

\[
\text{STAN_PROG}: \text{FUNCTIONS}?
\begin{align*}
\text{DATA}?
\text{TRANSFORMED\_DATA}?
\text{PARAMETERS}?
\text{TRANSFORMED\_PARAMETERS}?
\text{MODEL}?
\text{GENERATED\_QUANTITIES}?
\end{align*}
\]

Here ? indicates that the block may or may not be present.

Below is the syntax of the data block:
DATA: data { STMT_DECL;* }
STMT_DECL: TYPE identifier
TYPE: int | real | vector | matrix | ...

Here, identifier stands in for valid Stan variables names. The * symbols are Kleene stars to indicate an element that can be repeated or absent.

The parameters block is similar:

PARAMETERS: parameters { STMT_DECL;* }

The model block is more flexible:

MODEL: model { STMT_LPDF;* }
STMT_LPDF: STMT_BASIC
   | identifier ~ identifier( EXPR,* );
   | target+= EXPR;
STMT_BASIC: STMT_DECL | STMT_ASSIGNMENT | STMT_FOR
   | STMT_IFELSE | STMT_FUNCTION_APPLICATION | ...

Here, target is a reserved variable in Stan that represents the accumulated log-value of the density function.

STMT_BASIC and EXPR closely resemble C-like languages, so we omit their details here.

Stan allows user-defined function declared in the functions block:

FUNCTIONS: functions { FUNC_DECL* }
FUNCDECL: RET_TYPE identifier ((TYPE identifier),*) { STMT_FUNC;* }
STMT_FUNC: STMT_BASIC | return EXPR
RET_TYPE: TYPE | void

There are three more blocks:

TRANSFORMED_DATA: transformed data { STMT_BASIC;* }
TRANSFORMED_PARAMETERS: transformed parameters { STMT_LPDF;* }
GENERATED_QUANTITIES: generated quantities { STMT_BASIC;* }

The transformed data and transformed parameters blocks let users define transformed versions of the observed and hidden variables in a way that works efficiently with the inference process. The generated quantities block lets users define output quantities calculated from the samples of the parameters.

\[\text{Strictly speaking, we should not allow discrete types like int to be declared as parameters.}\]
3.2 Effects and Scope

Let $\text{Block}$ be the set of Stan block types, $\{\text{data, parameters, model,...}\}$.

Stan statements and expressions are sometimes allowed to be impure in particular ways depending which block contains that code. We call those impurities effects. We say that when code uses the random number generator, it has the $\text{RNG}$ effect, and when it increments the program’s density function with $\sim$ or target+= statements, it has the $\text{LPDF}$ effect. The set of effects $\text{Eff}$ is then $\{\text{RNG, LPDF}\}$. Stan’s specification implicitly defines a mapping $\text{effects}$ from some $\text{block} \in \text{Block}$ to the set of effects allowed within that block, $\text{effects}(\text{block}) \subset \text{Eff}$.

In Stan programs, the declarations that a statement may reference depends on the statement’s block and the declaration’s block. For instance, code in a transformed data block can reference top-level declarations in a data block but not in a parameters block. To know whether it is valid to inserting new statements into a given block, therefore, we need to know to which blocks’ declarations that statement is allowed to refer. Stan’s specification implicitly defines a mapping $\text{scope}$ from some $\text{block} \in \text{Block}$ to the set of blocks whose top-level declared variables statements that block may reference, $\text{scope}(\text{block}) \subset \text{Block}$.

3.3 Program validity

We define $\text{valid}_{\text{Stan}}$ to denote whether a program is valid, or roughly whether we expect it to compile. Let $\text{valid}_{\text{Stan}}(SP)$ for a Stan program $SP$ if and only if all of the following are true:

1. Effects and scopes of code are available in their block.

2. $SP$ typechecks as Stan code.

4 Modular Stan syntax

Below is an example modular Stan program:

data {
  int N;
  vector[N] x;
}
model {
  x ~ normal(Mean(), Stddev());
module "standard" Mean() {
    return 0;
}

module "standard" Stddev() {
    return 1;
}

module "normal" Mean() {
    parameters {
        real mu;
    }
    mu ~ normal(0, 1);
    return mu;
}

module "lognormal" Stddev() {
    parameters {
        real<lower=0> sigma;
    }
    sigma ~ lognormal(0, StddevInformative());
    return sigma;
}

module "yes" StddevInformative() {
    return 1;
}

module "no" StddevInformative() {
    return 100;
}

In the above program, the base is made up of the data and model blocks, Mean, Stddev and StddevInformative are holes, and each block starting with the keyword module are the module implementations.

The above modular Stan program has similar structure to the example in fig. 1. It also includes the example program section 3 as one of its nodes (where Mean is filled by normal, Stddev is filled by lognormal, and
Modular Stan makes two additions to Stan’s syntax: *Holes* and *module implementations*.

Holes are statements or expressions that are syntactically similar to function applications. We define variants of the Stan syntax rules that are allowed to include holes. For each Stan grammar rule `RULE` that can directly or indirectly contain a `STMT_BASIC`, `STMT_LPDF`, or `EXPR`, we define a new rule `RULE_M` that replaces those rules with the following `STMT_BASIC_M`, `STMT_LPDF_M`, and `EXPR_M` rules, respectively.

```stan
STMT_BASIC_M: hole_identifier(EXPR_M,*);
  | STMT_DECL | STMT_ASSIGNMENT_M | STMT_FOR_M
  | STMT_IFELSE_M | STMT_FUNCTION_APPLICATION_M | ...

STMT_LPDF_M: identifier ~ hole_identifier(EXPR_M,*);
  | identifier ~ identifier( EXPR_M,* );
  | target+= EXPR_M;
  | STMT_BASIC_M

EXPR_M: hole_identifier( EXPR_M,* ) | ...
```

We use `hole_identifier` to stand in for valid hole names.

Module implementations are reminiscent of function definitions, and appear at the top level alongside blocks:

```stan
MODULE_IMPLEMENTATION_M:
  module "impl_identifier" hole_identifier((TYPE identifier,)*) {
    PARAMETERS?
    STMT_LPDF_M;*
    return EXPR_M;*
  }
```

We use `impl_identifier` to stand in for valid implementation names, while `module` is a new keyword.

A modular Stan program is then:

```stan
MODULAR_STAN_PROG: STAN_PROG_M
  MODULE_IMPLEMENTATION_M*
```

We make two small additions to the syntax and capabilities of modular Stan in section 7 but this base syntax is sufficient to introduce its semantics and algorithms.
5 Modular Stan semantics

5.1 Basic operations on programs

We assume that there is some parsing procedure Parse such that, for all strings \( F \) of the language defined by the syntax in section 4, \( P = \text{Parse}(F) \), where \( P \) is some reasonable representation of \( F \) that we refer to loosely as a “modular Stan program”.

While the actual representation of a program \( P \) is an implementation detail, we can think of \( P \) as effectively a pair \( P = (P_{\text{base}}, \text{impls}(P)) \), where \( P_{\text{base}} \) represents the Stan-like base of \( P \) and \( \text{impls}(P) \) is the set of all module implementations defined in \( P \). \( P \) also implicitly includes the set of all holes referenced by \( P_{\text{base}} \) and \( \text{impls}(P) \).

We likewise are not concerned with the representations details of implementations or holes, we only need to define operations on them.

Below are the basic operations we use to interact with programs \( P \), implementations \( i \), holes \( h \), sets \( I \) of implementations, and sets \( H \) of holes:

- \( \text{impls}(h) \) is the set of implementations that implement a hole \( h \).
- \( \text{impls}(P) \) is the set of all implementations defined in \( P \).
- \( \text{impls}(H) = \bigcup_{h \in H} \text{impls}(h) \).
- \( \text{holes}(i) \) is the set of holes referenced in the definition of an implementation \( i \).
- \( \text{holes}(P_{\text{base}}) \) is the set holes referenced in the base of \( P \).
- \( \text{holes}(I) = \bigcup_{i \in I} \text{holes}(i) \).
- \( \text{holes}(P) = \text{holes}(P_{\text{base}}) \cup \text{holes}(\text{impls}(P)) \).
- \( \text{par}(i) \) is the hole that the implementation \( i \) implements, also called the parent of \( i \).
- \( \text{pars}(I) = \bigcup_{i \in I} \text{pars}(i) \).
- \( \text{pars}(P) = \text{pars}(\text{impls}(P)) \).

The above operations are specific to the context of a program \( P \). Since the intended \( P \) is usually clear, we only give the operation a subscript when disambiguation is necessary.
We note that \( \text{par} \) and \( \text{impls} \) operations are like inverses, so:

\[
i \in \text{impls}(h) \Leftrightarrow h \in \text{pars}(i)
\]

\[
h \in \text{pars}(I) \Leftrightarrow \exists i \in I \text{ s.t. } i \in \text{impls}(h)
\]

\[
i \in \text{impls}(H) \Leftrightarrow \exists h \in H \text{ s.t. } h = \text{par}(i)
\]

It is also be useful to note that, for all \( I_1 \subset I_2 \):

\[
\text{holes}(I_1) \subset \text{holes}(I_2)
\]

\[
\text{impls}(I_1) \subset \text{impls}(I_2)
\]

\[
\text{pars}(I_1) \subset \text{pars}(I_2)
\]

We also need to query certain syntactic elements of the code. Some of these operations are not fully detailed in the interest of brevity.

We call locations or spans \( \text{sites} \). We define a \( \text{HoleSite} \) as some data structure that captures the syntactic information of a hole called within code.

These are the operations on \( \text{HoleSites} \) \( hs \), programs \( P \), implementations \( i \), and blocks \( b \):

\( \text{sites}(i) \) or \( \text{sites}(P_{\text{base}}) \) is the set of hole sites in the code of \( i \) or \( P_{\text{base}} \), so that \( |\text{sites}(c)| \geq |\text{holes}(c)| \).

\( \text{sites}(P) \) is the set of hole sites in all of the code of \( P \).

\( \text{site}(b) \) is the site of the start of the code of block \( b \).

\( \text{block}(hs) \) is the block that contains \( hs \), if any.

\( \text{hole}(hs) \) is the hole that is called at \( hs \).

\( \text{scope}(i) \) is the set of blocks whose top-level declarations \( i \) references.

\( \text{effects}(i) \subseteq \text{Eff} \) is the set of effects whose top-level declarations \( i \) references.

We can syntactically break down implementations \( i \) into a triple, \((i_{\text{body}}, i_{\text{return}}, i_{\text{parameters}})\), so that:

\( i_{\text{body}} \) is the sequence of statements that makes of the code of the implementation,

\( i_{\text{return}} \) is the expression returned, if any,

\( i_{\text{parameters}} \) is the sequence of declarations of parameters made by the implementation.
5.2 Structural constraints

Not all modular Stan programs that can be parsed are valid; we also impose certain structural and semantic constraints. Input programs that do not meet the constraints are be rejected by the compiler.

Below are the structural constraints on a modular program $P$:

1. The dependency graph of modules is acyclic:
   
   For any graph $G$, let $N(G)$ be the set of nodes and $E(G)$ be the set of edges. Let the module dependency graph $MDG(P)$ be the directed graph with nodes $N(MDG(P)) = \text{impls}(P) \cup \{P_{\text{base}}\}$ and edges $E(MDG(P)) = \{ i_1 \rightarrow i_2 \mid i_1 \in \text{impls}(P) \cup \{P_{\text{base}}\}, i_2 \in \text{impls}(P), \text{par}(i_2) \in \text{holes}(i_1) \}$. We require that this graph is acyclic. We also refer to this property as $Acyclic(P)$.

2. Every hole has an implementation. $\forall h \in \text{holes}(P) \cup \text{holes}(P_{\text{base}})$, $\text{impls}(h) \neq \emptyset$.

3. Hole identifiers are unique and (hole identifier, implementation identifier) pairs are unique.

When a program $P$ meets these constraints, we say $valid_{\text{structure}}(P)$.

5.3 Module signatures and semantic constraints

5.3.1 Module Signatures

We would like to be able to guarantee that any concrete Stan program generated from a modular Stan program $P$ is valid. In order to do that, we need to understand the type, scope, and effect implications filling holes with their implementations.

To that end, we attempt to infer a signature for every hole in $P$. A signature is like a function type plus extra information. When no signature can be inferred for a hole, we reject the program as invalid. Signatures let us specify semantic constraints on input programs, and are also be useful for generating Stan programs in section 6.1.

A signature $s$ is a tuple:

$$s = (s_{\text{arg-types}}, s_{\text{ret-types}}, s_{\text{effects}}, s_{\text{scope}})$$

$s_{\text{arg-types}}$ specifies the argument types of a hole. $s_{\text{arg-types}}$ is a sequence of Stan types, like the TYPE syntactic element introduced in section 3.
\( s_{\text{ret-type}} \) specifies the return type of a hole. \( s_{\text{ret-type}} \) is a Stan return type, like the \textsc{RET\_TYPE} syntactic element introduced in section \( \text{section}\).

\( s_{\text{effects}} \) refers to the set of effects that a hole’s implementation may have.

\( s_{\text{scope}} \) refers to the scope of non-local variables that a hole’s implementation may reference.

1. Module Signature Inference

We define a procedure for either inferring the signature of a hole given the type determinations at each of the hole’s call sites and all of the hole’s implementations, or rejecting the program as invalid.

We rely on an operation \texttt{ReturnType} that infers the type of the expression returned by implementation code, if any, given that the types of all other expressions in that code are available. Type annotating is a standard operation for compilers of typed languages including the Stan compiler \[28\]. We use the following interface:

\[
\text{ReturnType}(\text{arguments}, i)
\]

where \texttt{arguments} is the collection of variable names and types available within the code of the implementation \( i \).

We visit each hole in topological order by dependency, such that when we visit a hole \( h \), for all \( i \in \text{impls}(h) \), all of the holes \( h' \in \text{holes}(i) \) have already been visited. This ordering is always possible because of the \textit{Acyclic}(P) property.

\[
\text{signature}(h) = (\text{argtypes}(\text{impls}(h)_0), \text{ReturnType}(\text{argtypes}(\text{impls}(h)_0), \text{impls}(h)_0, \bigcup_{i \in \text{impls}(h)} \text{effects}(i_{\text{body}}) \cup \bigcup_{h' \in \text{holes}(i)} \text{signature}(h')_{\text{effects}}, \bigcup_{i \in \text{impls}(h)} \text{scope}(i_{\text{body}}) \cup \bigcup_{h' \in \text{holes}(i)} \text{signature}(h')_{\text{scope}})
\]

\( \text{impls}(h)_0 \) is an arbitrary element of \( \text{impls}(h) \); \( \text{impls}(h) \) are never empty by structural constraint \[2\].

This way, \( s_{\text{arg-types}} \) is assigned to the argument types of any of its implementations, \( s_{\text{ret-types}} \) is assigned to the type that can be inferred from any of its implementations with the return types of dependent holes, and \( s_{\text{effects}} \) \( s_{\text{scope}} \) are the unions of the effects and scopes required by any of the hole’s implementations or descendants.
5.3.2 Semantic constraints

We give a set of semantic constraints on programs in terms of signatures:

1. Implementations match signature argtypes. \( \forall i \in \text{impls}(P), i_{\text{argtypes}} = \text{signature}(\text{par}(i))_{\text{argtypes}} \)

2. Implementations match signature rettype. \( \forall i \in \text{impls}(P), i_{\text{rettype}} = \text{signature}(\text{par}(i))_{\text{rettype}} \)

3. Effects and scopes of holes are available in their block or module signature. \( \forall i \in \text{impls}(P), \forall st \in \text{sites}(i): \)
   (a) \( \text{signature}(\text{st}_{\text{hole}})_{\text{effects}} \subseteq \text{signature}(\text{par}(i))_{\text{effects}} \)
   (b) \( \text{signature}(\text{st}_{\text{hole}})_{\text{scope}} \subseteq \text{signature}(\text{par}(i))_{\text{scope}} \)

4. Effects and scopes of code are available in their block or module signature.

5. \( P_{\text{base}} \) would typecheck under Stan if all holes \( h \) were function calls to function signatures with \( \text{signature}(h)_{\text{argtypes}} \) parameter types and \( \text{signature}(h)_{\text{rettype}} \) return type.

6. The body of each implementation \( i \) would typecheck under Stan if it were the body of a function with \( \text{signature}(\text{par}(i))_{\text{argtypes}} \) parameter types and \( \text{signature}(\text{par}(i))_{\text{rettype}} \) return type, and if the module-defined parameters \( i_{\text{parameters}} \) were included as model parameters.

When a program \( P \) meets these constraints, we say \( \text{valid}_{\text{semantics}}(P) \).

Constraint 6 defines the scope available to code within modules: local variables, module arguments, module-defined global variables (such as parameters), and base-defined global variables (such as parameters).

5.4 Program validity

We say that a modular Stan program \( P \) is valid if \( P \) meets both the structural constrains in section 5.3.2 and the semantic constraints in section 5.3.2: \( \text{valid}(P) = \text{valid}_{\text{structure}}(P) \land \text{valid}_{\text{semantics}}(P) \).
5.5 Selections

Selections are subsets of the implementations in a modular program. We call them “selections” because subsets of implementations are “selected” as components to build a concrete Stan model. When a selection specifies a Stan program and has no extra implementations, the selection is valid.

Next we give formal criteria to recognize valid selections, valid$_P(I)$. We show in section 6.1 that selections satisfying valid$_P(I)$ are exactly those needed to define concrete Stan programs. We first need to define siblings, an intersection-like operation on selections. siblings$(I_1, I_2)$ is the set of pairs of implementations across two sets that are different but share a parent:

$$siblings(I_1, I_2) = \{(i_1, i_2) \mid i_1 \in I_1, i_2 \in I_2, i_1 \neq i_2, \text{par}(i_1) = \text{par}(i_2)\}$$

We note a useful property:

$$I_1 \subseteq I_2 \implies \forall I', siblings(I_1, I') \subseteq siblings(I_2, I')$$

The property valid$_P(I)$ is true if and only if all of the following three criteria are met:

1. The selection only includes implementations that are in the program:

   $$I \subseteq \text{impls}(P)$$

2. Every hole in the program base and the selection has an implementation in the selection, and no extra implementations are included:

   $$\text{impls}(I) = \text{holes}(P_{\text{base}}) \cup \text{holes}(I)$$

3. The selection does not include any pair of implementations that implement the same hole, as these would be contradictory definitions:

   $$siblings(I, I) = \emptyset$$

The following are convenient restatements of the above properties 2 and 3:

1. Each hole found in the program base and the selection has exactly one implementation in the selection:

   $$\forall h \in \text{holes}(P_{\text{base}}) \cup \text{holes}(I), \mid \{i \mid i \in I, \text{par}(i) = h\} \mid = 1$$

2. $\forall h \in \text{pars}(I), h \in \text{holes}(I)$ or $h \in \text{holes}(P_{\text{base}})$.  

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5.6 Semantic domain

We are now equipped to formally define our high-level operations 1 to 3 and the semantic domain.

\textbf{Concretize} \((P, I)\) is the concrete Stan program that results from including each implementation from the set valid selection \(I\) into the base of the valid modular program \(P\). We consider an implementation of \textbf{Concretize} correct if for all modular programs \(P\) and selections \(I\) such that \(\text{valid}(P)\) and \(\text{valid}_I(P)\):

1. \(\text{valid}_{\text{STAN}}(\text{Concretize}(P, I))\)
2. \text{Concretize}(P, I) includes the same set of Stan statements in \(P_{\text{base}}\) and \(I\).

\textbf{ModelGraph}(\(P\)) is the graph of all valid selections of \(P\), connected if they disagree on implementation of one hole.

\[
N(\text{ModelGraph}(P)) = \{ I \mid I \in \text{impls}(P), \text{valid}_I(P) \}\]
\[
E(\text{ModelGraph}(P)) = \{ (I_1, I_2) \mid I_1, I_2 \in N(\text{ModelGraph}(P)), |\text{siblings}(I_1, I_2)| = 1 \}
\]

\textbf{ModelNeighbors} \((P, I)\) is the set of all selections that share an edge with \(I\) in the model graph: \(\text{ModelNeighbors}(P, I) = \{ I' \mid (I, I') \in E(\text{ModelGraph}(P)) \}\)

We can give a formal semantics of a valid modular program \(P\) in these terms: \([P]\) has the same graph structure as \(\text{ModelGraph}(P)\), but with the selection-valued nodes replaced by the corresponding probabilistic models:

\[
N([P]) = \{ [\text{Concretize}(P, I)] \mid I \in N(\text{ModelGraph}(P)) \}\]

In this way, a valid modular program \(P\) represents the graph of all probabilistic models that can be produced by recombination of modules, with connections between models that differ by only one choice of module.

6 Algorithms

6.1 Concretize

In this section we develop a function \textbf{Concretize}(\(P, I\)): the concrete Stan program that is derived from a modular Stan program \(P\) by applying the implementations of a valid selection set \(I\).

We build \textbf{Concretize} by careful use of function inlining as a subroutine. We use the following simplified interface:
InlineFunction(Program, CallSite, Stmts, Params)
InlineFunction(Program, CallSite, Stmts, Params, Return)

Here, Program is the whole program to be updated, CallSite is a data structure indicating the span of code to be replaced, Stmts are a list of statements that make up the body of the function, Params is a list of the function’s parameters, and Return, when present, is return expression (modules can only have zero or one return statements). When we use InlineFunction, we take Program to be a modular Stan program, CallSite to be a HoleSite, Stmts to be STMT_FUNC_M+, Params to be STMTDECL+, and Return to be EXPR_M.

InlineFunction is an operation standard in most optimizing compilers, including the Stan compiler [29].

InlineFunction assumes the following preconditions:

1. Program typechecks in the scope of CallSite.
2. CallSite supplies arguments matching Params.
3. The function represented by Stmts, Params and Return typechecks.

Then we assume the following properties of Program' = InlineFunction(Program, CallSite, Stmts, Params, Return):

1. References to Params in Stmts and Return are replaced by argument expression of CallSite.
2. Stmts are inserted in order before CallSite in the same scope as CallSite.
3. When Return is provided, CallSite is replaced by Return, which does not change the expression type.
4. Program' typechecks wherever Program typechecks.

6.1.1 ApplyImpl

We define an operation ApplyImpl(P, i), the result of taking a valid modular Stan program P and “applying” an implementation i ∈ impls(P), or using i to “fill” all instances of the hole par(i). The hole that i fills, par(i), no longer appears in the resulting program.
ApplyImpl(P, i):
  sites = \{ site \in HoleSites(p), site_{hole} = par(impl) \}
  P' := P
  for site in sites:
    P' := InlineFunction(P', site, i_{body}, signature(st_{hole})_{arg-types}, i_{return})
  return InlineFunction(P', site(\texttt{parameters}), \{\}, i_{parameters})

ApplyImpl does not update module signatures.

6.1.2 Correctness of ApplyImpl

Lemma 6.1 (ApplyImpl(P, i) replaces the hole filled by i with i’s holes). For all $i' \in \text{impls}(P) \cup \{P_{\text{base}}\}$, $\text{holes}_{\text{ApplyImpl}(P,i)}(i') = \text{holes}_P(i') \cup \text{holes}_P(i) - \{\text{par}(i)\}$ if $\text{par}(i) \in \text{holes}_P(i')$ and $\text{holes}_P(i')$ otherwise.

Proof. If $\text{par}(i) \notin \text{holes}_P(i')$, ApplyImpl does not make any replacements in $i'$, so $\text{holes}_{\text{ApplyImpl}(P,i)}(i') = \text{holes}_P(i')$.

Otherwise, ApplyImpl(P, i) is made up of code from i and $i'$, so:

\[
\text{holes}_{\text{ApplyImpl}(P,i)}(i') \subseteq \text{holes}_P(i) \cup \text{holes}_P(i')
\]

\[
= (\text{holes}_P(i) \cap \{\text{par}(i)\}) \cup (\text{holes}_P(i) - \{\text{par}(i)\})
\]

\[
\cup (\text{holes}_P(i') \cap \{\text{par}(i)\}) \cup (\text{holes}_P(i') - \{\text{par}(i)\})
\]

$\text{holes}_P(i) \cap \{\text{par}(i)\} = \emptyset$, because otherwise $i \rightarrow i \in E(MDG(P))$, which would violate Acyclic(P) and valid(P).

ApplyImpl replaces all $h \in \text{holes}_P(i') \cap \{\text{par}(i)\}$ with $i_{\text{body}}$, so $h \notin \text{holes}_{\text{ApplyImpl}(P,i)}(i')$.

Therefore:

\[
\text{holes}_{\text{ApplyImpl}(P,i)}(i') \subseteq (\text{holes}_P(i) - \{\text{par}(i)\}) \cup (\text{holes}_P(i') - \{\text{par}(i)\})
\]

ApplyImpl does not remove any $\text{holes}_P(i') - \{\text{par}(i)\}$, so $\text{holes}_P(i') - \{\text{par}(i)\} \subseteq \text{holes}_{\text{ApplyImpl}(P,i)}(i')$.

ApplyImpl inserts $\text{holes}_P(i) - \{\text{par}(i)\}$ as part of $i_{\text{body}}$, so $\text{holes}_P(i) - \{\text{par}(i)\} \subseteq \text{holes}_{\text{ApplyImpl}(P,i)}(i')$.

Therefore:

\[
\text{holes}_{\text{ApplyImpl}(P,i)}(i') = (\text{holes}_P(i) - \{\text{par}(i)\}) \cup (\text{holes}_P(i') - \{\text{par}(i)\})
\]

\[
= \text{holes}_P(i) \cup \text{holes}_P(i') - \{\text{par}(i)\}
\]

\[\square\]
Lemma 6.2 (ApplyImpl(P, i) replaces the hole filled by i with i’s holes). For all sites st ∈ sites(P) such that st_hole = par(i), the code i_body replacing st in ApplyImpl(P, i) has effects(i_body) ⊆ signature(par(i))_effects, scope(i_body) ⊆ signature(par(i))_scope, and for all holes h ∈ holes(i), signature(h)_effects ⊆ signature(par(i))_effects and signature(h)_scope ⊆ signature(par(i))_scope.

Proof. By definition of signature:

\[
signature(par(i))_effects \subseteq effects(i_body) \cup \bigcup_{h' \in \text{holes}(i)} \text{signature}(h')_effects
\]

and

\[
\text{signature}(par(i))_scope \subseteq \text{scope}(i_body) \cup \bigcup_{h' \in \text{holes}(i)} \text{signature}(h')_scope
\]

Lemma 6.3 (Preconditions of InlineFunction are met). When valid(P), the preconditions of the InlineFunction calls in ApplyImpl(P, i) are met.

Proof. Consider the first call:

\[\text{InlineFunction}(P, \text{site}, i_body, \text{signature}(st_hole)_arg-types, i\_return)\]

1. If site is in the base of P, then the P typechecks in the scope of site by semantic constraint 5, otherwise it must be in an implementation body, in which case it typechecks by semantic constraint 6.

2. We know site looks like a function call because of the definition of HoleSites. Its arguments must match signature(site_hole)_arg-types by semantic constraint 5.

3. Implied by semantic constraint 6.

On subsequent calls, P' is the output of a previous InlineFunction, which by induction meets its preconditions. P' typechecks by the same argument as P because of property 4. Both of the other preconditions hold by the same reasoning as the initial call.

Consider the final call:

\[\text{InlineFunction}(P', \text{site(parameters)}, \{\}, i\_parameters)\]
1. $P'$ typechecks at $\text{site(parameters)}$ because $P$ does by semantic constraint 5 and $P'$ typechecks wherever $P$ does.

2. $\text{site(parameters)}$ is a location rather than a hole site and so does not supply any arguments, which matches $\emptyset$.

3. $\text{Params}$ and $\text{Return}$ are empty, and $\text{Stmts}$ can only be a list of $\text{STMT\_DECL}$ and so typechecks.

\[\square\]

**Theorem 6.1** ($\text{ApplyImpl}$ produces valid modular Stan programs). $\text{valid}(P), i \in P \implies \text{valid}(\text{ApplyImpl}(P, i))$

**Proof.** Structural constraints:

1. **The dependency graph of modules is acyclic.**
   
   Suppose there is a cycle $C$ in $\text{MDG(ApplyImpl}(P, i)))$.
   
   Let $i_0 \rightarrow i_1$ be an edge in $C$; then $\text{par}(i_1) \in \text{holes}_{\text{ApplyImpl}(P, i)}(i_0)$.
   
   By Lemma 6.1, either $\text{par}(i_1) \in \text{holes}_{P}(i_0)$, in which case $i_0 \rightarrow i_1 \in E(\text{MDG}(P))$; or $\text{par}(i) \in \text{holes}(i_0)$ and $\text{par}(i_1) \in \text{holes}_{P}(i_0)$, in which case $i_0 \rightarrow i, i \rightarrow i_1 \in E(\text{MDG}(P))$.
   
   In either case, for all edges $i_0 \rightarrow i_1 \in C$, there exists a path from $i_0$ to $i_1$ in $\text{MDG}(P)$, so there exists a cycle in $\text{MDG}(P)$. As that would contradict $\text{valid}(P)$, there is no cycle $C$ in $\text{ApplyImpl}(P, i)$.

2. **Every hole has an implementation.**
   
   $\text{ApplyImpl}$ does not remove any implementations from or add any new holes to $P$, so any holes without implementations would also be without implementations in $P$, which would violate $\text{valid}(P)$.

3. **Hole identifiers are unique and (hole identifier, implementation identifier) pairs are unique.**
   
   $\text{ApplyImpl}$ does not change any hole implementation identifier names, so any collisions would exist in $P$ and violate $\text{valid}(P)$.

Semantic constraints:

1. **Implementations match signature argtypes.**
   
   $\text{ApplyImpl}$ does not change signatures or implementation argument types.
2. Implementations match signature rettype. ∀i′ ∈ impls(P), i′_rettype = signature(par(i′))_rettype.

If i_return is a hole expression of par(i), then it is replaced by ApplyImpl(P, i).
By Lemma 6.3 property 3 of InlineFunction for the replacement, so the type of i_return is not changed.

If the type of i_return depends on a hole expression of par(i), by the same reasoning, the type does not change. Otherwise, it is unaffected by ApplyImpl.

3. Effects and scopes of holes are available in their block or module signature.

Suppose ∃st ∈ sites(ApplyImpl(P, i)) so that st violates one of the conditions.

If st ∈ sites(P), since block and signature are unaffected by ApplyImpl, then st would violate valid(P). Therefore, st ∉ sites(P) and must have been part of a replacement of par(i) by i_body.

By Lemma 6.2 we have signature(st_hole)effects ⊆ signature(par(i))effects and signature(st_hole)scope ⊆ signature(par(i))scope. Since the scope and effects of st_hole are subsets of the scope and effects of par(i), and par(i) passes the four conditions, st_hole must also pass the four conditions.

4. Effects and scopes of code are available in their block or module signature.

By identical reasoning to the previous case, for any code in a block or module implementation, the code either existed in P, in which case it must be valid, or it replaced par(i), in which case by Lemma 6.2 it requires only a subset of the scope and effects of par(i), and is therefore also valid.

5. P_base would typecheck under Stan if all holes h were function calls to function signatures with signature(h)argtypes parameter types and signature(h)rettype return type.

By Lemma 6.3 property 4 of InlineFunction applies for all updates to P in ApplyImpl. Since P_base typechecks, ApplyImpl(P, i)_base also typechecks.

6. The body of each implementation i would typecheck under Stan if it were the body of a function signature(par(i))argtypes parameter types
and signature(par(i)) return type, and if the module-defined parameters i were included as model parameters.

By Lemma 6.2 property 4 of InlineFunction applies for all updates to i for any i ∈ impls(P) in ApplyImpl. Since i typechecks in P for all i ∈ impls(P), i also typechecks in ApplyImpl(P, i).

\[
\text{ApplyImpls}(P, I) = \text{ApplyImpl}(P, i) \quad \text{for each } i \in I.
\]

Formally, if we let \( I = \{i_1, \ldots, i_N\} \), \( P_0 = P \), and \( P_j = \text{ApplyImpl}(P_{j-1}, i_j) \) for \( j \in [1, N] \), then \( \text{ApplyImpls}(P, I) = P_N \).

6.1.3 ApplyImpls

Let \( \text{ApplyImpls}(P, I) \) be the result of applying \( \text{ApplyImpl}(P, i) \) for each \( i \in I \). Formally, if we let \( I = \{i_1, \ldots, i_N\} \), \( P_0 = P \), and \( P_j = \text{ApplyImpl}(P_{j-1}, i_j) \) for \( j \in [1, N] \), then \( \text{ApplyImpls}(P, I) = P_N \).

6.1.4 Correctness of ApplyImpls

**Theorem 6.2** (ApplyImpls(P, I) adds I’s holes and removes the holes filled by I). For all \( i' \in \text{impls}(P) \cup \{P_{\text{base}}\} \), \( \text{holes} \), \( \text{holes}_{\text{ApplyImpls}}(P, I)(i') \subset \text{holes}_P(i') \cup \text{holes}_P(I) - \text{pars}(I) \)

**Proof.** Let \( I = \{i_1, \ldots, i_j\} \) so that \( I_N = I \). Note that \( \text{ApplyImpls}(P, I_j) = P_j \).

We prove the following by induction on \( j \):

\[
\text{holes}_{P_j}(i') \subset \text{holes}_P(i') \cup \text{holes}_P(I_j) - \text{pars}(I_j)
\]

For \( j = 0 \): \( \text{holes}_{P_0}(i') \subset \text{holes}_P(i') \cup \text{holes}_{P_0}(I) - \text{pars}(I) = \text{holes}_P(i') \cup \emptyset = \text{holes}_{P_0}(i') \).

For \( j > 0 \): By Lemma 6.1 \( \text{holes}_{P_j}(i') = \text{holes}_{\text{ApplyImpl}(P_{j-1}, i_j)}(i') \subset \text{holes}_{P_{j-1}}(i') \cup \text{holes}_{P_{j-1}}(i_j) - \text{par}(i_j) \).

By induction:

\[
\text{holes}_{P_j}(i') \subset (\text{holes}_P(i') \cup \text{holes}_P(I_{j-1}) - \text{pars}(I_{j-1})) \cup \text{holes}_{P_{j-1}}(i_j) - \text{par}(i_j).
\]

Again by induction, we can use \( \text{holes}_{P_{j-1}}(i_j) \subset \text{holes}_P(i_j) \cup \text{holes}_P(I_{j-1}) - \text{pars}(I_{j-1}) \):

\[
\text{holes}_{P_j}(i') \subset (\text{holes}_P(i') \cup \text{holes}_P(I_{j-1}) - \text{pars}(I_{j-1})) \cup (\text{holes}_P(i_j) \cup \text{holes}_P(I_{j-1}) - \text{pars}(I_{j-1})) - \text{par}(i_j).
\]

\[
\text{holes}_{P_j}(i') \subset \text{holes}_P(i') \cup (\text{holes}_P(I_{j-1}) \cup \text{holes}_P(i_j) \cup \text{holes}_P(I_{j-1})) - (\text{pars}(I_{j-1}) \cup \text{par}(i_j)).
\]

\[
\text{holes}_{P_j}(i') \subset \text{holes}_P(i') \cup \text{holes}_P(I_j) - \text{par}(I_j).
\]
6.1.5 Concretize

We define Concretize as 
\[ \text{Concretize}(P, I) = \text{ApplyImpls}(P, I)_{\text{base}} \]
when \( I \) is a valid selection.

6.1.6 Correctness of Concretize

Lemma 6.4 (Concretize\((P, I)\) has no holes). For valid\((P)\) and valid\(_{P}(I)\),
\[ \text{holes}(\text{Concretize}(P, I)) = \emptyset. \]

Proof. By theorem 6.2, \( \text{holes}(\text{ApplyImpls}(P, I)_{\text{base}}) \subseteq \text{holes}(P_{\text{base}}) \cup \text{holes}(I) - \text{pars}(I) \). By valid\(_{P}(I)\), \( \text{holes}(P_{\text{base}}) \cup \text{holes}(I) = \text{pars}(I) \). Therefore, \( \text{holes}(\text{ApplyImpls}(P, I)_{\text{base}}) \subseteq \emptyset. \)

Theorem 6.3 (Concretize\((P, I)\) is a valid Stan program). valid\((P)\) and valid\(_{P}(I)\) implies valid\(_{\text{stan}}(\text{Concretize}(P, I))\).

Proof. By theorem 6.1 we have valid\((\text{ApplyImpls}(P, I))\).
By Lemma 6.4, we have \( \text{holes}(\text{Concretize}(P, I)) = \emptyset \). Therefore, \( SP = \text{Concretize}(P, I) \) is a concrete Stan program.
We can match the criteria of valid\(_{\text{stan}}(SP)\) in section 3.3:

1. Effects and scopes of code are available in their block. Implied by valid\((\text{ApplyImpls}(P, I))\), semantic constraint 4.

2. \( SP \) typechecks as Stan code. Implied by valid\((\text{ApplyImpls}(P, I))\), semantic constraint 5.

6.1.7 User specification of a selection

In order for a user to call Concretize, they need to provide a “selection”.

There is one more piece of syntax to define, though it does not appear in programs themselves: a selection string. A selection string is a string that references a set of module implementations within a given program.

SELECTION: hole_identifier:impl_identifier,+

Selection strings can be used to narrow down and index into the set of programs represented by a modular program.

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6.2 ModelGraph

In this section we present an efficient algorithm to implement the ModelGraph operation.

6.2.1 Naive versions

To demonstrate what we mean by efficient, consider a naive construction of the model graph given a modular program $P$:

$$N(\text{NaiveModelGraph}(P)) = \bigg\{ \text{close}(P_{\text{base}}, I) \bigg| I \in \bigtimes_{h \in \text{holes}(P)} \text{impls}(h), \text{valid}_P(\text{close}(P_{\text{base}}, I)) \bigg\}$$

$$E(\text{NaiveModelGraph}(P)) = \big\{ (I_1, I_2) \big| I_1, I_2 \in N(\text{NaiveModelGraph}(P)), |\text{siblings}(I_1, I_2)| = 1 \big\}$$

Here, $\text{close}(i, I)$ is the subset of $I$ that is reachable from $i$ by traversing edges in the module graph through $I$. Thus $\text{close}(P_{\text{base}}, I)$ effectively removes redundant implementations from $I$. \text{NaiveModelGraph} works by enumerating all possible combinations of implementations and model pairs and then filtering out the invalid options.

$E(\text{NaiveModelGraph}(P))$ is exponentially inefficient when $P$ is fig. 2a, because it would consider $2^N$ candidate neighbors for each node, where in reality each node has only $N - 1$ neighbors.

$N(\text{NaiveModelGraph}(P))$ is exponentially inefficient when $P$ is fig. 2b, because it would consider $2^N$ candidate nodes, where in reality there are only $N$ nodes.

Another approach would be a recursive construction. If the module graph is a tree, then the network of the sub-graph descending from each hole node is the graph join of the networks of the sub-graphs descending from its implementations, and the network of the sub-graph descending from each implementation node is the graph Cartesian product of the networks of the sub-graphs descending from its holes. The issue with this approach is how to handle situations like figs. 2c and 2d; the module graph is not always a tree, so hole and implementation nodes will sometimes combine networks with overlapping information. It is possible to modify the graph join and Cartesian product operations to handle the overlap correctly, but not without
Figure 2: Pathological module graphs. Round nodes represent the base and module implementations while rectangular nodes represent holes.
adding complexity and inefficiency that scales with the number recombination nodes.

6.2.2 Algorithm

Our algorithm builds up the model graph’s node and edge sets simultaneously by “visiting” each of the program’s holes in turn. The algorithm tracks the set of model and edge “prefixes”: partial selections that only contain implementations for the holes visited thus far. It also tracks the set of holes required so far by each prefix. When the algorithm “visits” a hole, it “expands” the set of prefixes that require that hole to reflect its set of implementations. To ensure that no “prefix” discovers that it requires a hole after that hole has been visited, and to avoid other complex edge cases, holes are visited in a topological order of dependency.

\[
\text{expand}(N, E, h) = \\
\left( \bigcup_{(H,I) \in N} \text{expand-node}(H, I, h), \right) \\
\bigcup_{(H,I) \in N} \text{new-edges}(H, I, h) \cup \bigcup_{(H_1,I_1,H_2,I_2) \in E} \text{expand-edge}(H_1, I_1, H_2, I_2, h) \right)
\]

\[
\text{expand-node}(H, I, h) = \\
\left\{ \begin{array}{ll}
\{(H \cup \text{holes}(i), I \cup \{i\}) | i \in \text{impls}(h)\} & \text{if } h \in H \\
\{(H, I)\} & \text{otherwise}
\end{array} \right.
\]

\[
\text{new-edges}(H, I, h) = \\
\left\{ \begin{array}{ll}
\{(H \cup \text{holes}(i_1), I \cup \{i_1\}, H \cup \text{holes}(i_2), I \cup \{i_2\}) | (i_1, i_2) \in \text{impls}(h)\} & \text{if } h \in H \\
\emptyset & \text{otherwise}
\end{array} \right.
\]

\[
\text{expand-edge}(H_1, I_1, H_2, I_2, h) = \\
\left\{ \begin{array}{ll}
\{(H_1, I_1, H_2, I_2)\} & \text{if } h \notin H_1, h \notin H_2 \\
\{(H_1 \cup \text{holes}(i), I_1 \cup \{i\}, H_2, I_2) | i \in \text{impls}(h)\} & \text{if } h \in H_1, h \notin H_2 \\
\{(H_1, I_1, H_2 \cup \text{holes}(i), I_2 \cup \{i\}) | i \in \text{impls}(h)\} & \text{if } h \notin H_1, h \in H_2 \\
\{(H_1 \cup \text{holes}(i), I_1 \cup \{i\}, H_2 \cup \text{holes}(i), I_2 \cup \{i\}) | i \in \text{impls}(h)\} & \text{if } h \in H_1, h \in H_2
\end{array} \right.
\]

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Let $G_{Dep}(P)$ be the graph of dependencies between holes of a program $P$ so that $N(G_{Dep}(P)) = \text{holes}(P)$ and $h_1 \rightarrow h_2 \in E(G_{Dep}(P))$ if and only if $\exists i \in \text{impls}(h_1)$ s.t. $h_2 \in \text{holes}(i)$. Let $\vec{H}$ be a topological ordering of $G(P)$.

Let $(N_0, E_0) = ((\text{holes}(P_{base}), \emptyset), \emptyset)$.

Let $(N_j, E_j) = \text{expand}(N_{j-1}, E_{j-1}, h_j)$, $\forall j \in [1, |\vec{H}|]$.

We show that $\{ I \mid (H, I) \in N_{|\vec{H}|} \} = N(\text{ModelGraph}(P))$ and $\{ (I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_{\vec{H}} \} = E(\text{ModelGraph}(P))$.

6.2.3 Proofs of correctness and completeness

Throughout this section, we assume that $P$ is a modular program such that $\text{valid}_{\text{structure}}(P)$.

Lemma 6.5 ($\vec{H}$ is ordered by dependency). There exists a topological ordering $\vec{H} = \text{topo}(G_{Dep}(P))$ and $\forall j \in [1, |\vec{H}|], \forall i \in \text{impls}(P)$ s.t. $\vec{H}_j \in \text{holes}(i), \text{par}(i) \in \vec{H}_{1:j-1}$ or $\text{par}(i) \in \text{holes}(P_{base})$.

Proof. The graph $G_{Dep}$ must be acyclic, because otherwise the holes of $P$ would have cyclic dependencies and $P$ would not be valid. Therefore $G_{Dep}$ has at least one topological order $\vec{H}$.

For any such $j$ and $i$, we must have $\text{par}(i) \rightarrow \vec{H}_j \in E(G_{Dep}(P))$, by definition of $G_{Dep}$. Then either $\text{par}(i) \in \text{holes}(P_{base})$ and we are done, or $\text{par}(i) \in \text{holes}(P)$, and so $\text{par}(i) \in \vec{H}$, so $\vec{H}_k$ for some $k$. By the definition of a topological ordering, $k < j$. Therefore, $\text{par}(i) \in \vec{H}_{1:j-1}$.

Lemma 6.6 (Model prefixes have complete prefix hole sets). $\forall j \in [1, |\vec{H}|], \forall (H_{j-1}, I_{j-1}) \in N_{j-1}$, let $N^I = \{ I' \mid I' \in N(\text{ModelGraph}(P)), I_{j-1} \subset I' \}$.

For all $I'$ in $N^I$, $\text{pars}(I') \cap \vec{H}_{1:j} = H_{j-1} \cap \vec{H}_{1:j}$.

Proof. This is a proof by induction on $j$.

We will simultaneously prove the following property, which we refer to as “consistency,” by induction for each $j$:

$I' \cap \text{impls}(\vec{H}_{1:j-1}) = I_{j-1} \cap \text{impls}(\vec{H}_{1:j-1})$

For $j = 1$:
Since $N_0 = \{ \emptyset \}$, $I_{j-1} = \emptyset$, so $N^I = N(\text{ModelGraph}(P))$.

If $\vec{H}_1 \in \text{pars}(I')$, then by $\text{valid}_P(I')$, $\vec{H}_1 \in \text{holes}(P_{base})$, since if $\exists i \in \text{impls}(I')$ s.t. $\vec{H}_1 \in \text{holes}(i)$, then by Lemma 6.5, $\text{par}(i) \in \vec{H}_{1:0} = \emptyset$. Then since $\text{holes}(P_{base}) \subset \text{pars}(I')$ and $H_0 = \text{holes}(P_{base})$, $\text{pars}(I') \cap \vec{H}_{1:1} = H_0 \cap \vec{H}_{1:1}$. 

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If $\vec{H}_1 \notin \text{pars}(I')$, then $\vec{H}_1 \notin \text{holes}(P_{\text{base}}) = H_0$, so $\text{pars}(I') \cap \vec{H}_{1:1} = H_0 \cap \vec{H}_{1:1} = \emptyset$. Therefore the lemma holds for $j = 1$.

Trivially, consistency holds for $j = 1$ because $\vec{h} \in \vec{H}_{1:0}$.

For $j > 1$:

Since $(H_{j-1}, I_{j-1}) \in N_{j-1}$ and $j \geq 2$, $\exists (H_{j-2}, I_{j-2}) \in N_{j-2}$ such that $(H_{j-1}, I_{j-1}) \in \text{expand-node}(H_{j-2}, I_{j-2}, \vec{H}_{j-1})$.

If $\vec{H}_{j-1} \in H_{j-2}$, then by induction of the lemma, $\vec{H}_{j-1} \in \text{pars}(I')$, so $I' \cap \text{impls}(\vec{H}_{j-1}) = \{i'\}$ for some $i'$. It also follows from the definition of $\text{expand-node}$ that, for some $i \in \text{impls}(\vec{H}_{j-1})$, $I_{j-1} = I_{j-2} \cup \{i\}$, and since $I_{j-2} \cap \text{impls}(\vec{H}_{j-1}) = \emptyset$, $I_{j-1} \cap \text{impls}(\vec{H}_{j-1}) = \{i\}$. Since $I_{j-1} \subset I'$, $i \in I'$.

If $i /\text{neg}$, then since $\text{par}(i) = \text{par}(i')$, $(i, i') \in \text{siblings}(I', I')$, but $\text{valid}_p(I')$ implies $\text{siblings}(I', I') = \emptyset$, so $i = i'$.

Thus, if $\vec{H}_{j-1} \in H_{j-2}$, then $I' \cap \text{impls}(\vec{H}_{j-1}) = I_{j-1} \cap \text{impls}(\vec{H}_{j-1}) = \{i\}$.

If $\vec{H}_{j-1} \notin H_{j-2}$, then $\vec{H}_{j-1} \notin \text{pars}(I')$ and $I_{j-1} = I_{j-2}$, so $I' \cap \text{impls}(\vec{H}_{j-1}) = I_{j-1} \cap \text{impls}(\vec{H}_{j-1}) = \emptyset$.

Starting from induction on consistency:

$$I' \cap \text{impls}(\vec{H}_{1:j-2}) = I_{j-2} \cap \text{impls}(\vec{H}_{1:j-2})$$

$$(I' \cap \text{impls}(\vec{H}_{1:j-2})) \cup (I' \cap \text{impls}(\vec{H}_{j-1})) = (I_{j-2} \cap \text{impls}(\vec{H}_{1:j-2})) \cup (I_{j-1} \cup \text{impls}(\vec{H}_{j-1}))$$

Because $I_{j-2} = I_{j-1} \cap \text{impls}(\vec{H}_{1:j-2})$:

$$(I' \cap \text{impls}(\vec{H}_{1:j-2})) \cup (I' \cap \text{impls}(\vec{H}_{j-1})) = (I_{j-1} \cap \text{impls}(\vec{H}_{1:j-2})) \cup (I_{j-1} \cup \text{impls}(\vec{H}_{j-1}))$$

$$I' \cap \text{impls}(\vec{H}_{1:j-1}) = I_{j-1} \cap \text{impls}(\vec{H}_{1:j-1})$$

Thus, consistency holds.

If $\vec{H}_{j} \in \text{holes}(P_{\text{base}})$, then the lemma is true by the same reasoning as the $j = 1$ case.

Suppose $\vec{H}_{j} \in H_{j-1}$ and $\vec{H}_{j} \notin \text{holes}(P_{\text{base}})$. By the construction of $H_{j-1}$ and the definition of $\text{expand-node}$, $\exists i \in I_{j-1}$ such that $\vec{H}_{j} \in \text{holes}(i)$.

If $I_{j-1} \subset I'$, $i \in I'$, so $\vec{H}_{j} = \text{par}(i) \in \text{pars}(I')$.

Suppose $\vec{H}_{j} \in \text{pars}(I')$ and $\vec{H}_{j} \notin \text{holes}(P_{\text{base}})$. By $\text{valid}_p(I')$ and Lemma 6.5 there exists some $k < j$ such that $\text{par}(i) = \vec{H}_k$ and $i \in \text{impls}(\vec{H}_k)$. By consistency, $I' \cap \text{impls}(\vec{H}_1:k) = I_k \cap \text{impls}(\vec{H}_1:k)$, so $i \in I_k \subset I_{j-1}$. By the definition of $\text{expand-node}(I_{j-1}, I_{j-1}, \vec{H}_k)$, $i \in I_k$ implies $\text{holes}(i) \subset H_k$, so $\vec{H}_{j} \in H_k \subset H_{j-1}$.

The following lemma shows that a model prefix can be expanded with any implementation on its horizon and remain a valid model prefix.
Lemma 6.7 (Model prefixes can be expanded with any implementation).
\( \forall j \in [1, |\vec{H}|], \forall I \in N(\text{ModelGraph}(P)), \forall h \in \text{holes}(I \cap \text{impls}(\vec{H}_{1,j}) \cup \text{holes}(P_{\text{base}})) - \vec{H}_{1,j}, \forall i \in \text{impls}(h), \exists I' \in N(\text{ModelGraph}(P)) \text{ s.t. } I \cap \text{impls}(\vec{H}_{1,j}) \cup \{i\} \subset I'. \)

Proof. We will construct a selection set that satisfies the property by modifying \( I \).

Let \( I_1 = I - \text{impls}(h) \cup \{i\} \). Let \( I_2 = I_1 \cup \{\text{any}(\text{impls}(h)) \mid h \in \text{holes}(P) - \text{pars}(I_2)\} \), where \( \text{any}(s) \) is an arbitrary element of a set. The sets \( \text{impls}(h) \) are never empty by \( \text{valid}(P) \). Then, \( \text{pars}(I_2) = \text{holes}(P) \) and \( I \cap \text{impls}(\vec{H}_{1,j}) \cup \{i\} \subset I_2 \).

Let \( f(I) = \{i \mid i \in I, \text{par}(i) \in \text{holes}(I) \cup \text{holes}(P_{\text{base}})\} \). Let \( I_3 \) be the fixed point applying \( f \) to \( I_2 \). We know \( f \) converges to some \( I_3 \) because \( |I| \) is finite, cannot go below \( 0 \), and decreases monotonically under \( f \) until convergence.

\( I_3 \) meets the criteria for \( \text{valid}_P(I_3) \):

1. \( I_3 \subset \text{impls}(P) : I_3 \subset I_1 \subset \text{impls}(\text{holes}(P)) \cup I \cup \{i\} \subset \text{impls}(P) \) by \( \text{valid}_P(I) \).

2. By \( I_3 = f(I_3) \) we know \( \text{pars}(I_3) \subset \text{holes}(I_3) \cup \text{holes}(P_{\text{base}}) \). Since \( \text{pars}(I_2) = \text{holes}(P) \supset \text{holes}(I_3) \cup \text{holes}(P_{\text{base}}) \) and \( f \) does not remove any \( h \in \text{holes}(I_3) \cup \text{holes}(P_{\text{base}}) \), we have \( \text{pars}(I_3) = \text{holes}(I_3) \cup \text{holes}(P_{\text{base}}) \).

3. \( \text{siblings}(I_3, I_3) = \emptyset \), because only one \( i \in \text{impls}(h) \) for each \( h \notin \text{pars}(I) \) is added to \( I \) in the construction of \( I_1 \) and \( I_2 \).

By construction, \( I \cap \text{impls}(\vec{H}_{1,j}) \cup \{i\} \subset I_3 \).

Lemma 6.8 (\( N_j \) represents exactly the model prefixes). \( \forall j \in [0, |\vec{H}|], \{I \mid (H, I) \in N_j\} = \{I \cap \text{impls}(\vec{H}_{1,j}) \mid I \in N(\text{ModelGraph}(P))\} \).

Proof. This is a proof by induction on \( j \).

For \( j = 0 \), \( \{I \mid (H, I) \in N_0\} = \{\emptyset\} = \{I \cap \emptyset \mid I \in N(\text{ModelGraph}(P))\} \).

For \( j \geq 1 \):

Suppose \( \exists I \in \{I \cap \text{impls}(\vec{H}_{1,j}) \mid I \in N(\text{ModelGraph}(P))\} \) such that \( I \notin \{I \mid (H, I) \in N_j\} \). Let \( I' = I \cap \text{impls}(\vec{H}_{1,j-1}) \). By induction, \( I' \in \{I \mid (H, I) \in N_{j-1}\} \), so \( \exists H', s.t., (H', I') \in N_{j-1} \).

If \( \vec{H}_j \in H' \), then by Lemma 6.6 \( \vec{H}_j \in \text{pars}(I) \), so \( \exists i \in I \text{ s.t. } i \in \text{impls}(\vec{H}_j) \).

By the definition of \( \text{expand-node}(H', I', \vec{H}_j) \), \( \forall i' \in \text{impls}(\vec{H}_j), I' \cup \{i'\} \in \{I \mid (H, I) \in N_j\} \), so \( I' \cup \{i\} = I \in \{I \mid (H, I) \in N_j\} \), which contradicts the construction of \( I \).

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If $\vec{H}_j \neq H'$, then by Lemma 6.6, $\vec{H}_j \neq pars(I)$, so $I' = I$. By the definition ofexpand-node($H', I', \vec{H}_j$), $(H', I') \in N_j$, so $I \in \{I \mid (H, I) \in N_j\}$, which
again contradicts the construction of $I$.

Therefore, there is no such $I$, and $\{I \cap impls(\vec{H}_{1:j}) \mid I \in N(ModelGraph(P))\} \subset
\{I \mid (H, I) \in N_j\}$.

Suppose $\exists I \in \{I \mid (H, I) \in N_j\}$ such that $I \notin \{I \cap impls(\vec{H}_{1:j}) \mid I \in
N(ModelGraph(P))\}$. By the definition of $N_j$, $\exists (H', I') \in N_{j-1} \text{ s.t. } (H, I) \in
expand-node(H', I', \vec{H}_j)$. By induction, $I' \in \{I \cap impls(\vec{H}_{1:j-1}) \mid I \in
N(ModelGraph(P))\}$, and therefore $\exists I^* \in N(ModelGraph(P)) \text{ s.t. } I' \subset I^*$.

If $\vec{H}_j \neq H'$, then by the definition ofexpand-node, $I = I'$, and by
Lemma 6.6, $\vec{H}_j \neq pars(I^*)$; so $I = I' = I^* \cap impls(\vec{H}_{1:j-1}) = I^* \cap
impls(\vec{H}_{1:j})$, so $I \in \{I \cap impls(\vec{H}_{1:j}) \mid I \in N(ModelGraph(P))\}$.

If $\vec{H}_j \neq H'$, then by the definition ofexpand-node, $\exists i \in impls(\vec{H}_j)$ s.t. $I = I' \cup \{i\}$, and by Lemma 6.6, $\vec{H}_j \neq pars(I^*)$.

Because $\vec{H}_j \in holes(I^* \cap impls(\vec{H}_{1:j-1})) - \vec{H}_{1:j-1}$, by Lemma 6.7, $\exists i \in
N(ModelGraph(P)) \text{ s.t. } I \cap impls(\vec{H}_{1:j-1}) \cup \{i\} \subset I^i$, so $I' \cup \{i\} = I \subset I^i$,
so $I \in \{I \cap impls(\vec{H}_{1:j}) \mid I \in N(ModelGraph(P))\}$.

Therefore, $\{I \mid (H, I) \in N_j\} \subset \{I \cap impls(\vec{H}_{1:j}) \mid I \in N(ModelGraph(P))\}$.

\[ \Box \]

**Theorem 6.4** ($N_{|\vec{H}|}$ is correct and complete). $\{I \mid (H, I) \in N_{|\vec{H}|}\} = N(ModelGraph(P))$.

**Proof.** By Lemma 6.8, $\{I \mid (H, I) \in N_{|\vec{H}|}\} = \{I \cap impls(\vec{H}_{1:|\vec{H}|}) \mid I \in
N(ModelGraph(P))\}$, and because $\vec{H}_{1:|\vec{H}|} = pars(P)$, $\{I \cap impls(\vec{H}_{1:|\vec{H}|}) \mid I \in
N(ModelGraph(P))\} = N(ModelGraph(P))$. \[ \Box \]

**Lemma 6.9** (Edge prefix endpoints are model prefixes). $\forall j \in [0, |\vec{H}|], \forall (H_1, I_1, H_2, I_2) \in E_j$, $(H_1, I_1) \in N_j$ and $(H_2, I_2) \in N_j$.

**Proof.** This is a proof by induction on $j$.

For $j = 0$, the lemma is trivially satisfied because $E_0 = \varnothing$.

For $j \geq 1$:

By definition ofexpand, $(H_1, I_1, H_2, I_2)$ came either from new-edges?

If $(H_1, I_1, H_2, I_2) \in new-edges(H', I', \vec{H}_j)$ for some $(H', I') \in N_{j-1}$, then
$\vec{H}_j \in H'$ and $(H_1, I_1) = (H' \cup holes(i_1), I' \cup \{i_1\})$, $(H_2, I_2) = (H' \cup
holes(i_2), I' \cup \{i_2\})$, so $(H_1, I_1), (H_2, I_2) \in expand-node(H', I', \vec{H}_j) \subset N_j$.

If $(H_1, I_1, H_2, I_2) \in expand-edge(H'_1, I'_1, H'_2, I'_2, \vec{H}_j)$ for some $(H'_1, I'_1, H'_2, I'_2) \in
E_{j-1}$, then by induction $(H'_1, I'_1), (H'_2, I'_2) \in N_{j-1}$. If $\vec{H}_j \in H'_1$, then $\exists i \in
E_{j-1}$.
impls(H'_1) s.t. (H_1, I_1) = (H'_1 \cup \text{holes}(i_1), I'_1 \cup \{i_1\}) \in \text{expand-node}(H'_1, I'_1, \bar{H}_j) \subset N_j. \text{ If } \bar{H}_j \notin H'_1, \text{ then } (H_1, I_1) = (H'_1, I'_1) \in \text{expand-node}(H'_1, I'_1, \bar{H}_j) \subset N_j.

The same reasoning applies for (H_2, I_2).

Lemma 6.10 (Edge prefix endpoints share one pair of siblings). \( \forall j \in [0, |\bar{H}|], \forall (H_1, I_1, H_2, I_2) \in E_j, |\text{siblings}(I_1, I_2)| = 1. \)

Proof. This proof by induction on \( j \).

For \( j = 0 \), the lemma is trivially satisfied because \( E_0 = \emptyset \).

For \( j \geq 1 \):

By definition of \text{expand-edge}, \( (H_1, I_1, H_2, I_2) \) came either from \text{new-edges} expand-edge.

If \( (H_1, I_1, H_2, I_2) \in \text{new-edges}(H', I', \bar{H}_j) \) for some \( (H', I') \in N_{j-1} \), then

\[ \exists (i_1, i_2) \in \binom{\text{impls}(\bar{H}_j)}{2} \text{ such that } I_1 = I' \cup \{i_1\}, I_2 = I' \cup \{i_2\}, \text{par}(i_1) = \text{par}(i_2) = \bar{H}_j, \text{so } (i_1, i_2) \in \text{siblings}(I_1, I_2). \]

Since \( I_1 \) and \( I_2 \) are otherwise identical, \text{siblings}(I_1, I_2) \) can have no other elements.

If \( (H_1, I_1, H_2, I_2) \in \text{expand-edge}(H'_1, I'_1, H'_2, I'_2, \bar{H}_j) \) for some \( (H'_1, I'_1, H'_2, I'_2) \in E_{j-1} \), then by induction \text{siblings}(I'_1, I'_2) = \{ (i_1, i_2) \} \) for some \( i_1, i_2 \).

Since \( (I_1, I_2) \) is either \( (I'_1, I'_2) \) or \( (I'_1 \cup \{i\}, I'_2 \cup \{i\}) \) for some \( i \in \text{impls}(\bar{H}_j) \), \( I_1 \) and \( I_2 \) cannot have gained or lost any siblings, so \text{siblings}(I_1, I_2) = \{ (i_1, i_2) \} \).

Lemma 6.11 (Model prefixes without siblings are equal). \( \forall I_1, I_2 \in N(\text{ModelGraph}(P)), \forall j \in [1, |\bar{H}|], \) let \( I'_1 = I_1 \cap \text{impls}(\bar{H}_{1:j}) \) and \( I'_2 = I_2 \cap \text{impls}(\bar{H}_{1:j}). \)

If \text{siblings}(I_1, I_2) = \emptyset, then \( I'_1 = I'_2. \)

Proof. Let \( i \) be the element of \( I'_1 - I'_2 \) so that \( \text{par}(i) = \bar{H}_k \) with minimal \( k \).

Since \( i \notin I'_2 \) and \text{siblings}(I'_1, I'_2) = \emptyset, \( \bar{H}_k \notin \text{pars}(I'_2). \)

Since \text{valid}_P(I_1) \) and \( \bar{H}_k \in \text{pars}(I'_1), \bar{H}_k \in \text{holes}(P_{\text{base}}) \cup \text{holes}(I'). \)

Since \text{valid}_P(I_2), \text{holes}(P_{\text{base}}) \subset \text{pars}(I'_2), \text{so } \bar{H}_k \notin \text{holes}(P_{\text{base}}), \text{so } \exists i' \in I'_1 \text{ s.t. } \bar{H}_j \in \text{holes}(i'). \)

By the topological sorting of \( \bar{H}_j \), \( \text{par}(i') = H_m \) for some \( m < k \). Since \( k \) is minimal in \( I'_1 - I'_2 \), \( i' \neq I'_1 - I'_2 \), so \( i' \notin I'_2 \). Then \( \bar{H}_k \in \text{holes}(i') \subset \text{holes}(I'_2) \subset \text{pars}(I'_2) \), but \( \bar{H}_k \notin \text{pars}(I'_2). \)

Therefore \( I'_1 - I'_2 \) is empty. The same reasoning applies to show \( I'_2 - I'_1 \) is empty, so \( I'_1 = I'_2. \)

Lemma 6.12 (\( E_j \) is a complete set of edge prefixes). \( \forall j \in [1, |\bar{H}|], \{ (I_1 \cap \text{impls}(\bar{H}_{1:j}), I_2 \cap \text{impls}(\bar{H}_{1:j})) \mid I_1, I_2 \in N(\text{ModelGraph}(P)), \text{siblings}(I_1, I_2) = \{ (i_1, i_2) \}, \text{par}(i_1) \in \bar{H}_{1:j} \} \subset \{ (I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_j \}. \)

Proof. This is a proof by induction on \( j \).

For \( j = 0 \), \( \{ (I_1 \cap \emptyset, I_2 \cap \emptyset) \mid I_1, I_2 \in N(\text{ModelGraph}(P)), \text{siblings}(I_1, I_2) = \{ (i_1, i_2) \}, \text{par}(i_1) \in \emptyset \} = \emptyset \subset E_0 = \emptyset. \)
For $j \geq 1$:

We consider some $(I_1, I_2) \in \{(I_1 \cap \impls(H_{1:j}), I_2 \cap \impls(H_{1:j})) \mid I_1, I_2 \in N(\text{ModelGraph}(P)), \text{siblings}(I_1, I_2) = \{(i_1, i_2)\}, \text{par}(i_1) \in H_{1:j}\}$ and show that $(I_1, I_2) \in \{(I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_j\}$. Let $\{(i_1, i_2)\} = \text{siblings}(I_1, I_2)$.

If $\text{par}(i_1) = \text{par}(i_2) = \vec{H}_j$, then since $\text{siblings}(I_1 - i_1, I_2 - i_2) = \emptyset$, by Lemma 6.11, $I_1 - i_1 = I_2 - i_2$. Since $I_1 - i_1 \subset \impls(H_{1:j-1})$, by Lemma 6.8, $\exists H' \text{ s.t. } (H', I_1 - i_1) \in N_{j-1}$, therefore \textup{new-edges}(H', I_1 - i_1, \vec{H}_j) \subset E_j$, and because $\vec{H}_j \in \text{pars}(I_1)$ implies $\vec{H}_j \in H'$ and $(i_1, i_2) \in (\impls(H_j))^2$, $(H' \cup \text{holes}(i_1), I_1 - i_1 \cup i_1 = I_1, H' \cup \text{holes}(i_2), I_1 - i_1 \cup i_2 = I_2) \in \text{new-edges}(H', I_1 - i_1, \vec{H}_j)$.

If $\text{par}(i_1) = \text{par}(i_2) \neq \vec{H}_j$, then by induction, $(I_1 \cap \impls(H_{1:j-1}), I_2 \cap \impls(H_{1:j-1})) \in \{(I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_{j-1}\}$, so $\exists (H'_1, I'_1, H'_2, I'_2) \in E_{j-1}$ such that $I'_1 = I_1 \cap \impls(H_{1:j-1})$ and $I'_2 = I_2 \cap \impls(H_{1:j-1})$.

If $\vec{H}_j \notin H'_1$ and $\vec{H}_j \notin H'_2$, then by Lemma 6.9 and Lemma 6.6, $I_1 = I'_1, I_2 = I'_2$, and by the definition of expand-edge, $(H'_1, I'_1, H'_2, I'_2) = (H'_1, I'_1, H'_2, I'_2, \vec{H}_j) \subset E_j$.

If $\vec{H}_j \in H'_1$ and $\vec{H}_j \notin H'_2$, then $\exists i \in \impls(\vec{H}_j)$ such that $I_1 = I'_1 \cup \{i\}$ and $I_2 = I'_2$, and $\forall i' \in \impls(\vec{H}_j)$, $(H'_1 \cup \text{holes}(i'), I'_1 \cup \{i\}, H'_2, I'_2) = (H'_1 \cup \text{holes}(i'), I_1, H'_2, I_2) \in \text{expand-edge}(H'_1, I'_1, H'_2, I'_2, \vec{H}_j) \subset E_j$. Similarly, if $\vec{H}_j \notin H'_1$ and $\vec{H}_j \in H'_2$, then $I_1 = I'_1, I_2 = I'_2 \cup \{i\}$ and $(H'_1, I'_1, H'_2 \cup \text{holes}(i), I'_2 \cup \{i\}) = (H'_1, I_1, H'_2 \cup \text{holes}(i), I_2) \in \text{expand-edge}(H'_1, I'_1, H'_2, I'_2, \vec{H}_j) \subset E_j$.

If $\vec{H}_j \in H'_1$ and $\vec{H}_j \in H'_2$, then since $\text{par}(i_1) \neq \vec{H}_j$, $\exists i \in \impls(\vec{H}_j)$ such that $I_1 = I'_1 \cup \{i\}$ and $I_2 = I'_2 \cup \{i\}$, and $\forall i' \in \impls(\vec{H}_j)$, $(H'_1 \cup \text{holes}(i), I'_1 \cup \{i\}, H'_2 \cup \text{holes}(i), I'_2 \cup \{i\}) = (H'_1 \cup \text{holes}(i), I_1 \cup \{i\}, H'_2 \cup \text{holes}(i), I_2) \in \text{expand-edge}(H'_1, I'_1, H'_2, I'_2, \vec{H}_j) \subset E_j$.

\textbf{Theorem 6.5} \textit{(E_{\vec{H}}) is the correct and complete edge set).} $\{(I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_{\vec{H}}\} = E(\text{ModelGraph}(P))$.

\textbf{Proof.} $\forall (H_1, I_1, H_2, I_2) \in E_{\vec{H}}$, by Lemma 6.9, so $I_1, I_2 \in N(\text{ModelGraph}(P))$ by theorem 6.4 and also $|\text{siblings}(I_1, I_2)| = 1$ by Lemma 6.10. Therefore $(I_1, I_2) \in E(\text{ModelGraph}(P))$, so $\{(I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_{\vec{H}}\} \subset E(\text{ModelGraph}(P))$. 

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Because $\vec{H}_{1:|\vec{H}|} = \text{pars}(P)$,

$$
\begin{align*}
\left\{ (I_1 \cap \text{impls}(\vec{H}_{1:|\vec{H}|}), I_2 \cap \text{impls}(\vec{H}_{1:|\vec{H}|})) \mid I_1, I_2 \in N(\text{ModelGraph}(P)), \\
\text{siblings}(I_1, I_2) = \{(i_1, i_2)\}, \\
\text{par}(i_1) \in \vec{H}_{1:|\vec{H}|} \right\}
\end{align*}
$$

$$
= \{(I_1, I_2) \mid I_1, I_2 \in N(\text{ModelGraph}(P)), |\text{siblings}(I_1, I_2)| = 1 \}
$$

$$
= E(\text{ModelGraph}(P))
$$

So by Lemma 6.12, $E(\text{ModelGraph}(P)) \subset \left\{ (I_1, I_2) \mid (H_1, I_1, H_2, I_2) \in E_{|\vec{H}|} \right\}$

6.2.4 Efficiency

For a modular program $P$, let $N = |N(\text{ModelGraph}(P))|$ and $E = |E(\text{ModelGraph}(P))|$. Index the graph nodes as $\{ n_i \mid i \in [1..N] \} = N(\text{ModelGraph}(P))$ and the edges as $\{(e_{i,1}, e_{i,2}) \mid i \in [1..E] \} = E(\text{ModelGraph}(P))$. Let $H = |\text{holes}(P)|$.

The minimum size possible of the explicit representation of $\text{ModelGraph}(P)$ is then $\sum_{i \in [1..N]} |n_i| + \sum_{j \in [1..E]} |e_{j,1}| + |e_{j,2}|$ identifiers.

1. **Runtime efficiency.** Consider the selection set insertion operations $I \cup \{i\}$ in expand-node. Since implementations are never removed from any selection sets, and selection sets are never removed from model prefix sets, the number of such insertions must be $O(\sum_{i \in [1..N]} |n_i|)$.

Consider the hole union operations $H \cup \text{holes}(i)$ in expand-node. Since each $h \in \text{holes}(i)$ is eventually replaced by exactly one implementation, the amortized cost is again $O(\sum_{i \in [1..N]} |n_i|)$.

The same arguments apply to the edge operations in new-edges and expand-edge: the number of implementation set insertions must be $O(\sum_{j \in [1..E]} |e_{j,1}| + |e_{j,2}|)$, and the amortized cost of each hole union operation is also $O(\sum_{j \in [1..E]} |e_{j,1}| + |e_{j,2}|)$.

The set inclusion checks $h \in H$ result in a small constant overhead for expand-node, new-edges and expand-edge. Since expand is called $H$ times with at most $N$ nodes and $E$ edges, the number of inclusion checks is $O(H \times N + H \times E)$.

The resulting runtime complexity is then $O(H \times N + H \times N)$.  

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2. **Space efficiency.** Because the nodes \( N_j \) and edges \( E_j \) are the entire program state, \(|N_j| \leq |N(\text{ModelGraph}(P))|\) and \(|E_j| \leq |E(\text{ModelGraph}(P))|\), and the elements of \( N_j \) and \( E_j \) are less than or equal to the elements of \( N(\text{ModelGraph}(P)) \) and \( E(\text{ModelGraph}(P)) \), the program state never exceeds the size of the output, so space complexity is \( \Theta(\sum_{i \in [1...N]} |n_i| + \sum_{j \in [1...E]} |e_{j,1}| + |e_{j,2}|) \).

3. **Notes on efficiency.** Since \( N_H \) does not depend on any \( E_j \), when we only calculate the graph nodes we have a runtime complexity of \( O(H \cdot \sum_{i \in [1...N]} |n_i|) \) and space complexity of \( O(\sum_{i \in [1...N]} |n_i|) \).

This method can efficiently handle the extreme cases in fig. 2. We have no no asymptotic time or space overhead for the example fig. 2b, and for fig. 2a, we have no space overhead but an asymptotic time overhead of \( O(H \cdot H) \) set inclusion checks.

6.3 **ModelNeighbors**

Let \( Nei(I, P) \) be a shorthand for our previously defined ModelNeighbors:,

\[
Nei(I, P) = \text{ModelNeighbors}(P, I) = \{ I' \mid (I, I') \in E(\text{ModelGraph}(P)) \}.
\]

Let \( \text{Limit}(I, P) \) be equal to a modular program \( P \), except that, for all holes \( h \in \text{pars}(P) \):

\[
\text{impls}_{\text{Limit}(I, P)}(h) = \begin{cases} 
\text{impls}_P(h) \cap I & \text{if } h \in \text{pars}(I) \\
\text{impls}_P(h) & \text{otherwise}
\end{cases}
\]

We can compute \( Nei \) efficiently with \( \text{Limit} \) and our previously defined ModelGraph algorithm:

\[
Nei(I, P) = \bigcup_{i \in I} \bigcup_{i' \in \text{impls}(\text{par}(i)) \cup \{i\}} N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P)))
\]

6.3.1 **Proofs of correctness and completeness**

**Lemma 6.13** (\( \text{Limit}(I, P) \) is a valid modular program). \( \text{valid}_{\text{structure}}(P) \), \( \text{valid}_P(I) \) implies \( \text{valid}_{\text{structure}}(\text{Limit}(P, I)) \).

**Proof.** Requirements 1 and 2 are implied by \( \text{valid}_{\text{structure}}(P) \) and \( \text{impls}(\text{Limit}(P, I)) \subset \text{impls}(P) \).

Requirement 3 is \( \forall h \in \text{holes}(P) \cup \text{holes}(P_{\text{base}}), \text{impls}_{\text{Limit}(P, I)}(h) \neq \emptyset \). For every \( h \), if \( h \notin \text{pars}(I) \), then \( \text{impls}_{\text{Limit}(P, I)}(h) = \text{impls}_P(h) \).
which must be non-empty given \( \text{valid}_{\text{structure}}(P) \). If \( h \in \text{pars}(I) \), then \( \text{impls}_{\text{Limit}(P,I)}(h) = \text{impls}_P(h) \cap I \), which must have one element by the definition of \( \text{valid}_P(I) \).

**Lemma 6.14** (Neighbors of \( I \) are valid under \( \text{Limit}(I - \{i\} \cup \{i'\}, P) \)). \( \forall I' \in N(\text{ModelGraph}(P)) \) such that \( \text{siblings}(I, I') = \{(i, i')\}, \text{valid}_{\text{Limit}(I - \{i\} \cup \{i'\}, P)}(I') \).

**Proof.**

1. \( I' \subset \text{impls}(\text{Limit}(I - \{i\} \cup \{i'\}, P)) \): Suppose \( \exists i' \in I' \) such that \( i' \notin \text{impls}(\text{Limit}(I - \{i\} \cup \{i'\}, P)) \). It must be that \( \text{par}(i') \notin \text{impls}(\text{Limit}(I - \{i\} \cup \{i'\}, P)) \), because otherwise \( \text{impls}_{\text{Limit}(I - \{i\} \cup \{i'\}, P)}(i') = \text{impls}_P(i') \) by the definition of \( \text{Limit} \). Then \( \exists i' \in I - \{i\} \cup \{i'\} \) s.t. \( \text{par}(i') = \text{par}(i') \), so \( (i', i') \in \text{siblings}(I - \{i\} \cup \{i'\}, I') \) and \( (i', i') \notin (i, i') \).

Since \( i' \in I', i' \neq i' \), so \( i' \in I' \). Then \( (i', i') \in \text{siblings}(I, I') \), which contradicts \( \text{siblings}(I, I') = \{(i, i')\} \), so there is no such \( i' \).

2. \( \text{pars}(I') = \text{holes}(I') \cup \text{holes}(\text{Limit}(I - \{i\} \cup \{i'\}, P)_{\text{base}}) \) follows from \( \text{valid}_P(I') \) and Lemma 6.13 because \( \text{Limit} \) does not modify \( \text{base}, \text{holes} \) or \( \text{pars} \).

3. \( \text{siblings}(I', I') = \emptyset \) by \( \text{valid}_P(I') \).

**Lemma 6.15** (Selections that are valid under \( \text{Limit}(I - \{i\} \cup \{i'\}, P) \) are neighbors of \( I \)). \( \forall I' \in N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P))) \), \( \text{valid}_P(I') \) and \( \text{siblings}(I, I') = \{(i, i')\} \).

**Proof.** Because \( \text{impls}(\text{Limit}(I - \{i\} \cup \{i'\}, P)) \subset \text{impls}(P) \) and Lemma 6.13, \( \text{valid}_{\text{Limit}(I - \{i\} \cup \{i'\}, P)}(I') \) implies each requirement of \( \text{valid}_P(I') \).

Suppose \( \text{siblings}(I, I') = \emptyset \). Because \( I, I' \in N(\text{ModelGraph}(P)) \), by Lemma 6.11, \( I = I' \). Then, \( i \in I \implies i \in I' \). However, by \( \text{valid}_{\text{Limit}(I - \{i\} \cup \{i'\}, P)}(I') \), \( I' \subset \text{impls}(\text{Limit}(I - \{i\} \cup \{i'\}, P)) \neq i \), which is a contradiction. Therefore \( \text{siblings}(I, I') \neq \emptyset \).

Let \( (i_2, i_2') \in \text{siblings}(I, I') \), so \( \text{par}(i_2) = \text{par}(i_2') \). If \( \text{par}(i_2') \neq \text{par}(i) \), then by the definition of \( \text{Limit} \), \( \text{impls}_{\text{Limit}(I - \{i\} \cup \{i'\}, P)}(i_2') = \{i_2\} \), so \( i_2 = i_2' \), which contradicts \( (i_2, i_2') \in \text{siblings}(I, I') \). If \( \text{par}(i_2') = \text{par}(i) \), then \( \text{impls}_{\text{Limit}(I - \{i\} \cup \{i'\}, P)}(i_2') = \{i'\} \), so \( (i_2, i_2') \) must be \( (i, i') \). Therefore, \( \text{siblings}(I, I') = \{(i, i')\} \).
Theorem 6.6 (The models of \( \text{Limit}(I - \{i\} \cup \{i'\}, P) \) are exactly the neighbors of \( I \) with \( \text{siblings}(I, I') = \{i, i'\} \), so we can union over possible siblings).

\[
\text{Nei}(I, P) = \bigcup_{i \in I} \bigcup_{i' \in \text{impls}(\text{par}(i)) - \{i\}} N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P)))
\]

Proof. By Lemmas 6.14 and 6.15, \( \{ I | I \in N(\text{ModelGraph}(P)), \text{siblings}(I, I') = \{(i, i')\} \} = N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P))) \).

\[
\bigcup_{i \in I} \bigcup_{i' \in \text{impls}(\text{par}(i)) - \{i\}} N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P)))
\]
\[
= \bigcup_{i \in I} \bigcup_{i' \in \text{impls}(\text{par}(i)) - \{i\}} \{ I | I \in N(\text{ModelGraph}(P)), \text{siblings}(I, I') = \{(i, i')\} \}
\]
\[
= \{ I | I \in N(\text{ModelGraph}(P)), |\text{siblings}(I, I')| = 1 \}
\]
\[
= \text{Nei}(I, P)
\]

\[
\]

6.3.2 Efficiency

Since we are using the \text{ModelGraph} implementation from section 6.2.2, the runtime complexity of \( N(\text{ModelGraph}(P)) \) is \( O(H * N) \) for \( H = \text{holes}(P) \) and \( N = |N(\text{ModelGraph}(P))| \).

Our runtime complexity is then:

\[
O(\text{Nei}(I, P)) = O\left( \bigcup_{i \in I} \bigcup_{i' \in \text{impls}(\text{par}(i)) - \{i\}} N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P))) \right)
\]
\[
= O\left( \sum_{i \in I} \sum_{i' \in \text{impls}(\text{par}(i)) - \{i\}} N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P))) \right)
\]
\[
= O\left( \sum_{i \in I} \sum_{i' \in \text{impls}(\text{par}(i)) - \{i\}} H |N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P)))| \right)
\]
\[
= O\left( H \sum_{i \in I} \sum_{i' \in \text{impls}(\text{par}(i)) - \{i\}} |N(\text{ModelGraph}(\text{Limit}(I - \{i\} \cup \{i'\}, P)))| \right)
\]
\[
= O\left( H |\text{Nei}(I, P)| \right)
\]

Our space complexity is the size of the output.
7 Additional features

This section presents two extensions of the module system described in sections 4 and 5, giving users more expressive power to build their desired networks of models.

7.1 Append blocks

In the base syntax, we allow modules to define a parameters block that upon concretization is appended onto the base parameters block. In the same way, we can allow modules to add on to each of the other Stan blocks (except for data, which is fixed for the whole network of models). The extended syntax generalizes MODULE_IMPLEMENTATION_M:

\[
\text{MODULE_IMPLEMENTATION_M:}
\text{module "impl_identifier" hole_identifier((TYPE identifier,)*) {}
  \text{FUNCTIONS_M?}
  \text{TRANSFORMED_DATA_M?}
  \text{TRANSFORMED_PARAMETERS_M?}
  \text{PARAMETERS?}
  \text{MODEL_M?}
  \text{GENERATED_QUANTITIES_M?}
  \text{STMT_LPDF_M;*}
  \text{return EXPR_M;?}
}\]

We refer to these module blocks as append blocks because they are appended to the end of their corresponding Stan blocks upon concretization.

The rules for scope and available effects are the same for within-module blocks as they are for the corresponding Stan blocks as described in section 3.2. For example, variables defined in a module transformed parameters block can be referenced inside of that module’s model block but not its transformed data block. Module arguments are not available inside append blocks.

ApplyImpl is updated to include InlineFunction calls for each append block in the same way that it is used for parameters.

Concretization is still correct:

- Scope is preserved: For any statement in a module that could reference a global variable \( g \) in module append block \( B \), \( g \) will still be a valid reference after concretization because \( B \) must also be included. For any
statement $S$ in a module append block that references a global variable $h$ in its corresponding base block, $h$ will still be a valid reference after concretization because $M$ will be inserted after the declarations of the base block.

- Type correctness and effect correctness are preserved because appends are statements and must have the same effect requirements as the blocks into which they are inserted, as usual.

- All other arguments about statement order, well-typedness, and lack of cycles are unaffected by this change.

Since the inclusion of append blocks has no affect on the module dependency graph, this change does not change the correctness of the network of models or neighbor algorithms.

Use cases of append blocks include:

- Defining functions for use in the module and as arguments to its descendants.

- Defining transformed data or transformed parameters that are used in the module.

- Adding a prior distribution to the model block for each parameter defined the module, without requiring that the module signature have the LPDF effect.

- Emitting the likelihood of the data under a distribution defined the module as a generated quantity (as in the case study in section 9.3).

### 7.2 Module fields

Sometimes, two or more behaviors only make sense to include together.

For example, suppose we want to define a change of variables transformation. We need to define a transform function and corresponding inverse function. Suppose we want to abstract the transformation into a hole so that it can be swapped out. If we were to define separate holes for Transform and Inverse, we may end up with implementations may not match, because they can be selected independently. We would rather have one hole, Transformation, that packages compatible transform and inverse implementations together.

We can achieve this coupling by letting modules contain multiple named behaviors call fields. With fields, we would defined one hole, Transformation,
with two fields, `forward` and `reverse`, referenced in code as `Transformation.forward` and `Transformation.reverse`.

Fields of a module also share the append blocks (and therefore global scope) of a module.

The syntax for associated behavior introduces a second, optional variant of `MODULE_IMPLEMENTATION_M` where arguments are moved into field declarations:

```
MODULE_IMPLEMENTATION_M: module "impl_identifier" hole_identifier {  
  FUNCTIONS_M?  
  TRANSFORMED_DATA_M?  
  TRANSFORMED_PARAMETERS_M?  
  PARAMETERS?  
  MODEL_M?  
  GENERATED_QUANTITIES_M?  

  field field_identifier?(TYPE identifier*) {  
    STMT_LPDF_M;*  
    return EXPR_M;*  
  } +  
}
```

We use `impl_identifier` to stand in for valid field names, while `field` is a new keyword.

Each of a hole’s fields must be implemented by a corresponding field block and implementations as though it were a new hole. A field $f_1$ in hole $h$ is referenced as $h.f_1(\ldots)$, except when the field identifier $f_1$ is empty, in which case the reference is $h(\ldots)$.

Each of a hole’s fields is treated like a separate hole for the purposes of concretization, and they have no differences in terms of the correctness of the resulting Stan program. Holes with fields are treated like holes without fields for the purpose of building the module graph, model graph and neighbor sets; an implementation has a dependency on a hole $h$ if any of its fields depends on $h$.

Coupling behavior into the fields of a module is only one constraint that we could impose on co-selection of implementations. We discuss a more general constraint logic in section [10].
8 Macros

While the module system described so far is in theory flexible enough to describe arbitrarily complex networks of models, it may sometimes be too verbose to be practical.

For instance, suppose we want to build a regression model, but we don’t know which of \(N\) features to include. Our model space of interest then consists of one model for each subsets of features. Since we want to choose inclusion or exclusion for each feature, we will need at least \(N\) holes, each with two implementations, so we will need to write \(2^N\) implementations. This is cumbersome and repetitive for large \(N\).

To make the language more expressive, we define a series of “macros” as shorthand ways of generating larger modular programs. Each macro is translated by the compiler back into the basic module language, so we can then use the same algorithms defined in section 6.

Table 1 is a summary of the macros described in the following sections.

| Name              | Syntax   | Description                                                                 |
|-------------------|----------|-----------------------------------------------------------------------------|
| Collection hole   | \(H^+\) | Select a subset of implementations rather than one                           |
| Indexed hole      | \(H[i..j]\) | Copy implementations of \(H\) for each index in range                        |
| Hole instance     | \(H<j>\) | Copy a hole; same selection but new parameters                               |
| Hole copy         | \(H<e>\) | Copy a hole; independent selection                                           |
| Ranged versions   | \(H<i..j>\) | Apply the macro for each index in range, collecting an array of results      |
| Multi-ranges      | \(i..j,k..l,\ldots\) | Same as a range, but for each index combination                           |
| Range exponent    | \((i..j)^e\) | Same as a range, but \(e\) indices without replacement                   |
| Hole product      | \(H_1\,*H_2\) | New hole with implementations \(impls(H_1) \times impls(H_2)\)           |
| Hole exponent     | \(H^j\) | Same as a hole product but without replacement                             |

Table 1: Summary of macros

The expansion of each macro transforms the program’s module graph in some way, it may synthesize new modules with new (Stan) code, and it may define a translation of selection strings (section 6.1.7) to apply to the post-expansion module graph.

8.1 Collection holes

A “collection hole” is a hole that can be filled with any number of implementations, rather than exactly one.
Consider our regression model example where we want to use a subset of $N$ features. For each feature, we need a hole with one implementation that includes the feature and another that does not. Then, we need to collect all of the holes into an array to pass into the regression. The “collection hole” macro automates this pattern, so that the user can instead write one “collection hole” with $N$ implementations instead of $N$ holes and $2N$ implementations.

Collection holes are identified by a $+$ at the end of a hole identifier. The value of a non-void collection hole is an array containing the values of the selected implementations in an undefined order.

Figure 3 shows how expansion of collection holes modifies a program’s module graph.

Figure 3: Collection hole module graph transformation. A collection hole $H+$ produces a modified hole that lets a user select which implementations to include (yes) or exclude (no), and then concatenates the results ($H_{merge}$).

For each implementation $i$ of $h+$, the implementation yes is the same as $i$ but wraps its result in a singleton array, while no does nothing and returns an empty list. The implementation $merge_h$ returns a concatenation of the arrays returned by each new hole.

Users can then select a subset of implementations in their selection strings, as in $..h: [i_1, i_2, ..]..$. If a collection hole $h$ has a set of implementations $C$, then a selection string $s_{before}, h: [I], s_{after}$ for some list of implementations $I \subset C$ is translated to $s_{before}, h: merge_h, \bigcup_{i \in I} h_i:yes$, $\bigcup_{i \in C-I} h_i:no$, $s_{after}$.

The network produced by a collection hole includes an edge between two nodes if they differ by exactly one inclusion.

---

3Like a Hamming graph.
8.2 Indexed holes

An “indexed hole” is a hole that can generate additional implementations.

Indexed holes are identified by adding a range \([i..j]\), where \(i\) and \(j\) are non-negative integer literals, to the end of a hole identifier. Implementations of indexed holes accept an index as an extra argument, denoted in brackets at the end of the hole identifier in their definition, such as in `module "i" h[j](..) {..}`. Here, \(j\) is the index, and can be used as an integer literal within the module, because it will be replaced with each integer in the range upon macro expansion. In this way, each written module implementation serves as a template for generating more.

Figure 4 shows how expansion of indexed holes modifies a program’s module graph.

![Indexed hole module graph transformation. An indexed hole \(H[i..N]\) produces \(N\) copies of its implementation.](image)

Users can then specify an indexed implementation to fill the indexed hole, as in `..h:i[5]..`

8.3 Hole instances and hole copies

So far, the design of holes effectively assumes that they represent decisions about individual subcomponents of a model. For example, when a parameter is defined within a hole, it is only ever translates to single parameter in the resulting program. It may be instead that a hole should be repeated in multiple places.

For example, suppose a hole \(h\) represents a model of a storm cloud. What if we have data from two storm clouds? There are three possibilities:

1. We only want one copy of \(h\), and data from both clouds will be used to estimate the parameters in \(h\).
2. We want two copies of \( h \), one to model each cloud, with identical implementations but separate parameters.

3. We want two copies of \( h \), one to model each cloud, but which may have different implementations.

Case 1 corresponds to the basic semantics: users can call \( h() \) multiple times, but all references to \( h \) are filled with the same implementation, and the append blocks of \( h \)'s implementation are only added once, so all references use the same parameters.

Case 2 is the motivation for a macro called **hole instances**.

Case 3 is the motivation for a macro called **hole copies**.

### 8.3.1 Hole instances

Hole instances are identified by the syntax `hole_identifier<j>`, where \( j \) is a non-negative integer literal. Hole instances are transformed in the module tree in the following way:

Figure 5 shows how expansion of hole instances modifies a program’s module graph.

![Figure 5: Hole instance module graph transformation. When some code \( p_i \) refers to \( H<i> \), a new hole called \( H<i> \) is created with copies of the implementations of \( H \). Here, \( h[1] \ldots h[N] \) are identical copies of \( h \) except that their local and global variables are given unique names. This way, there are \( N \) copies of the implementation of \( h \), each referring to its own set of new global variables such as parameters. Each \( j \) found in a reference `hole_identifier<j>` produces a new instance.

Users specify selections in the same way as if \( h \) were not copied: \( \ldots, h:i, \ldots \). A selection string \( s_{before}, h:i, s_{after} \) is translated into \( s_{before}, \bigcup_{j=1\ldots N} h:j:i, s_{after} \).

Optionally, module implementations can accept an index as an extra argument, denoted in angle brackets at the end of the hole identifier in their definition, such as in `module "i" h<j>(\ldots) {\ldots}`. When that module
implementation is used as a hole instance, the variable \( j \) can be used as an integer literal. This way, \( j \) can specify hole instances within the module, copying deeper into the module graph.

8.3.2 Hole copies

Hole copies are identified by the syntax `hole_identifier\{j\}`, where \( j \) is a non-negative integer literal. Hole copies behave the same way as hole instances, except that implementations must be selected independently for each generated hole `h\{j\}`, as in: `..., h\{1\}:i_1, ..., h\{N\}:i_N, ...`

8.3.3 Ranged hole instances and copies

To generate many hole instances or copies automatically, `h[1:N](..)` is translated into a Stan array `{ h[1](..), h[2](..), ..., h[N](..) }` and `h<1:N>(..)` is translated into `{ h<1>(..), h<2>(..), ..., h<N>(..) }`.

8.4 Multi-ranges and range exponents

Macros that can have ranges, namely `H[i..j]`, `H<i..j>`, and `H\{i..j\}`, can also accept multi-ranges. Multi-ranges are the same as ranges except that they produce one result per combination of their ranges. For example, a `1..3,1..5` produces `(1,1), (1,2), .. (3,5)`. Implementations that accept indices as extra arguments, such as `h\{j\}`, must then accept `h<i,j>`.

Ranges exponents come in three variants. `R^n` is equivalent to a multi-range with \( R \) repeated \( n \) times, for example, `(1..3)^2` is equivalent to `1..3,1..3`. `R^P^n` is like `R^n` except that it gives ordered permutations without replacement, for example `(1..3)^P3` does not include `(1,1), (2,2), or (3,3)`. `R^C^n` is like `R^P^n` except that it gives unordered combinations without replacement, for example `(1..3)^C3` does not include `(2,1), (3,1), or (3,2)`. Multi-ranges and range exponents make it easier to generate holes and implementations that represent combinations.

8.5 Hole products and hole exponents

A hole product `H_1*H_2(., .)` is a hole that combines the implementations of the holes `H_1` and `H_2`. For each \( i_1 \in \text{impls}(H_1) \) and \( i_2 \in \text{impls}(H_2) \), \((i_1, i_2)\) is an implementation of `H_1 \times H_2` that returns a tuple of the results of `i_1` and `i_2`. The arguments lists of `H_1` and `H_2` are concatenated together to make the argument list of `H_1*H_2`.
Figure 6 shows how expansion of hole products modifies a program’s module graph.

![Figure 6: Hole product expansion shown as a module graph transformation.](image)

When some code $p$ refers to a product $H_1 \ast H_2$, a new hole is created with the cartesian product of $H_1$ and $H_2$’s implementations.

Hole exponents are analogous to range exponents from section 8.4. $H^n$ is equivalent to the product of $H$ with itself $n$ times. $H^P_n$ gives the ordered $n$-permutations of $impls(H)$ without replacement, while $H^C_n$ gives the unordered $n$-combinations of $impls(H)$ without replacement.

### 8.6 Example application of macros

Recall the regression example in which we want to include some subset of $N$ variables in our model. Suppose $N = 100$. To encode this model space in the module system requires $2N = 200$ module implementations. Using an indexed collection hole, we can reduce this to one handwritten module implementation.

```plaintext
data {
    int N;
    matrix[100, N] x;
    vector[N] y;
}
parameters {
    real sigma;
}
model {
    y ~ normal(sum(Feature[1..100]+(x)), sigma);
}
module "f" Feature[n](x) {
    parameters {
```

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This program represents a family of regression models on $y$ given the features $x$, each including a different subset of features. $y$ is modeled with a normal distribution centered on the sum of the subset of features, $\text{Feature}[1..100]+(x)$, which is an indexed collection hole: the range $[1..100]$ copies the Feature module implementation for $n=1$ to 100, and the $+$ indicates that each implementation is either included or excluded from the result. An individual Stan program can be generated from this family by supplying a selection string, such as: $\text{Feature}:[1,2,3]$, which includes only the first three features.

Now suppose we also want our regression to include some subset of 2- and 3-way interactions between variables, such as $x[3]*x[9]$ or $x[4]*x[10]*x[99]$. To encode this model space requires $2*(100 + \binom{100}{2} + \binom{100}{3}) = 333500$ module implementations. We can use macros to reduce this to two or three handwritten module implementations. We will show two alternative implementations.

The first way makes use of range exponents:

data {
  int N;
  matrix[100, N] x;
  vector[N] y;
}
parameters {
  real sigma;
}
model {
  y ~ normal(sum( Feature[1..100]+(x) )
              + sum( FeaturePair[(1..100)^C2]+(x) ),
              + sum( FeatureTriplet[(1..100)^C3]+(x) ),
              sigma);
}

module "f" Feature[n](x) {
  parameters {
    real theta;
  }
  return theta * x[n];
module "fp" FeaturePair[n, m](x) {
  parameters {
    real theta;
  }
  return theta * x[n] .* x[m];
}

module "ft" FeatureTriplet[n, m, p](x) {
  parameters {
    real theta;
  }
  return theta * x[n] .* x[m] .* x[p];
}

This program uses indexed collection holes with range exponentials to collect and sum a subset of the features, feature pairs, and feature triplets. An individual Stan program can be generated by supplying a selection string such as:

Feature: [1,2,3], FeaturePair: [(1,2),(1,4)], FeatureTriplet: [(1,2,3),(4,10,99)]

The second way makes use of hole products and exponents:

data {
  int N;
  matrix[100, N] x;
  vector[N] y;
}

parameters {
  real sigma;
}

model {
  vector[N] total = rep_vector(0, 100);
  for ((t, r) in Theta*Col[1..100]+()) {
    total += t * r;
  }
  for ((t, r1, r2) in Theta*Col[1..100]-C2+()) {
    total += t * r1 .* r2;
  }
  for ((t, r1, r2, r3) in Theta*Col[1..100]-C3+()) {
    total += t * r1 .* r2 .* r3;
  }
}
y ~ normal(total, sigma);
}

module "t" Theta() {
    parameters {
        real theta;
    }
    return theta;
}

module "r" Col[n]() {
    return x[n];
}

By taking a product Theta*Col[1..100], we are generating an implementation of Col for each index 1 to 100, and then producing a new parameter for each of those implementations. By taking a product of Theta with the exponent Col[1..100]^2, we are producing a new parameter for each pair of indices. Each of these products returns an array of tuples of values which must then be multiplied and summed into the total vector. The selection strings for this program look like: Theta*Col:\[(t,1),(t,2),(t,3)\], Theta*Col^2:\[(t,1,2),(t,1,4)\], Theta*Col^3:\[(t,1,2,3),(t,4,10,99)\].

These programs have \(\approx 333500\) module implementations and represent networks with \(2^{100} + {100 \choose 2} + {100 \choose 3} \approx 10^{50000}\) models. How can we use such large programs and spaces? By never explicitly representing them. Macros instantiate synthetic modules lazily, only when they are selected. Large networks can be explored efficiently by only enumerating neighbors with ModelNeighbors; in this case, the network diameter and branching factor are a more manageable 166750.

9 Example case studies

In this section we present two small but real-world probabilistic modeling case studies that we have translated into the modular Stan language, and we discuss their benefits. These case studies showcase only two of the motivating use cases listed in section 1; the rest we for future work.

In addition, we present a web interface that can be used to follow along with our two examples.
9.1 Interactive web interface

We have built a prototype web interface for development and interactive visualizations of modular Stan [21]. Figure 7 shows its interface.

![Prototype of a modular Stan interface](image)

Figure 7: A labeled screenshot of the prototype web interface for modular Stan.

Users can write a modular Stan program or load an example program and compile it at (a). When they do, interactive visualizations are produced: (b) the module graph and (c) the model graph.

The page keeps track of a module selection set. Users can modify the selection by: selecting or deseleting implementations the module graph (b), selecting complete models in the model graph (c), editing the selection string directly (d), or selecting a previously labeled model (d). When the selection is modified, the model graph (c) highlights nodes compatible with that selection, and when the selection is valid, the corresponding concrete Stan program is displayed (e) and labels and notes associated with that program can be edited (f). The set of model labels and notes can be saved and loaded as a text file.

Users can also bookmark and annotate nodes in model graph. Annotations can be saved and loaded as files separate from the modular Stan file, in a format that maps between the model’s unique selection set and model labels and annotations.

Interactive versions of the following two case studies can be found at [34](#).
and [31].

9.2 “Golf” case study: Modular Stan for ease and clarity of development

This section gives a basic demonstration of how modular Stan can cleanly support and express a typical model development workflow, as an example of application 3.

The “Golf” case study [32] follows the development of a Bayesian statistical model for describing the probability that a professional golfer will sink a shot given their distance from the hole.

We represent the modeling process as a single modular Stan program. The base of the program is the part that remains constant throughout development:

```stancode
data {
  int J; // Number of distances
  vector[J] x; // Distances
  int n[J];  // Number of shots at each distance
  int y[J];  // Number of successful shots at each distance
}
model {
  y ~ NSuccesses(n, PSuccess(x));
}
```

The `data` block describes `J` distances, where the `j`th distance is `x[j]` feet, and `y[j]` shots out of `n[j]` were successful.

The `model` block describes an abstracted modeling approach: we model the number of successes `y` as being drawn from some distribution `NSuccesses` parameterized by the number of attempts `n` and the probability of success `PSuccess`, which itself is a function of the distance `x`. `NSuccesses` and `PSuccess` are holes.

A natural distribution to choose for `NSuccesses` is the binomial distribution. We express this as a module:

```stancode
module "binomial" NSuccesses(y | n, p) {
  y ~ binomial(n, p);
}
```

A simple way to take a real value like `x` to a probability is the `logit` function, so we choose to explore that option first for `PSuccess`:

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module "logistic" PSuccess(x) {
    parameters {
        real a;
        real b;
    }
    return logit(a + b*x);
}

If we stop here, we have only one choice of implementation for each of our holes, so our modular Stan program defines only one valid Stan program:

data {
    int J; // Number of distances
    vector[J] x; // Distances
    int n[J]; // Number of shots at each distance
    int y[J]; // Number of successful shots at each distance
}
parameters {
    real a;
    real b;
}
model {
    y ~ binomial(n, logit(a + b*x));
}

This program implement logistic regression, which is the first model explored in the case study.

The next step in the probabilistic workflow or Box's loop is to criticize our model by applying it to the data. We find that the model fit is lacking and the parameters a and b have no obvious physical interpretation.

This criticism motivates us to try a more sophisticated, more physically realistic implementation for PSuccess. If we suppose that a shot will be successful if its trajectory angle is sufficiently precise, and we suppose that the angle is normally distributed, then we can write our model in terms of angle variance:

// A shot's angle is good if the center of the ball would roll over the hole.
module "angle_success" PSuccess(x) {
    parameters {

real sigma_angle;
}
real r = (1.68 / 2) / 12; // ball radius
real R = (4.25 / 2) / 12; // hole radius
vector[J] threshold_angle = asin((R-r) ./ x);
vector[J] p_angle = 2*Phi(threshold_angle / sigma_angle) - 1;
return p_angle;
}

We find this model has superior fit and interpretability and we continue iterating by adding on modules in this fashion.

The completed representation of the case study can be found with our source code [33] or at the web interface along with visualizations [34]. Here it is presented by the web interface:

Though this is a small example, we already see some benefits to clarity:

- There is only a single, minimal source file;
- We have a standard, integrated way to draw the development path and document the decision-making evidence and rationale at each step;
- The modular organization makes the solution space easier to understand and extend.

9.3 “Birthday” case study: Modular Stan as a platform for automation

This section gives an example of how the network of models provides a platform for automation (use case [1]). We demonstrate constructing a network,
defining an evaluation metric, and performing a simple graph search. We use a moderately sized network of models from a case study of incremental model improvements. This approach would also apply to other multiple-model contexts, such as feature selection and symbolic regression.

The “Birthday” case study [35, 36] follows the development of a statistical model of the number of babies born in the US on a given day, given birth data from 1969-1988. The authors used a time-series Gaussian process approach. Like many probabilistic modeling case studies and publications, the Birthday case study presents a series of models that differ by incremental variations. The authors explicitly evaluate nine models, but the model variations they present implicitly define a much larger set of models that it would be reasonable to explore: what if a different combination of variations were applied, or in a different way? To feasibly explore that larger set of models, we need automation, and for automation, we need an explicit representation of the model space, like the network of models offered by a modular Stan program.

We start by translating the case study into a single modular Stan program. The translation reduces the number of lines of code from 1098 to 270 while increasing the number of models represented from nine to 120.

The translation process is largely mechanical, and involves encapsulating the variation between the given models into modules. For example, model 2 adds a days-of-the-week Gaussian process component onto model 1, model 3 adds a long-term-trend component onto model 2, etc. Each of these variations becomes one or more module in the modular Stan program. The full translation of the modular program can be found with our source code [30] or at the web interface along with visualizations [31].

Figure 9 shows the model graph produced by the modular program. To automatically search these 120 models for high-quality options, we must first define “quality” by choosing a model-scoring metric. One reasonable approach is to measure a model’s predictive accuracy by computing its Expected Log-Posterior Density (ELPD). ELPD approximates the leave-one-out prediction accuracy of a model for a dataset [37].

While ELPD is relatively efficient, it could still take a long time to accurately compute ELPD for every model in our network. Our goal, then, is to find high-quality models with as few ELPD evaluations as possible. Here we take the simplest approach, a greedy graph search, and leave more

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4Our modular Stan program would have been significantly more concise if we used the collection hole feature described in section 8.1, but they were not implemented in our prototype compiler at the time of writing.
Figure 9: The model graph corresponding to the Birthday problem modular Stan program. Each node represents a model and each edge represents one swapped-out module.
sophisticated search methods for future work.

Our greedy graph search loops over the following steps, given an arbitrary starting point:

1. Score the neighbors of the current model.

2. Move to the highest scoring model seen so far, or if that is the current model, return it.

This search algorithm is not guaranteed to be optimal; it is analogous to a gradient descent of a (likely non-convex) space. Intuitively, the closer the maximal-neighbor operation is to a gradient, the more efficient the search will be, so we can expect that the semantically minimal changes represented by the edges in the model graph provide exactly the topology of models closest to a smooth continuous space.

The search algorithm is implemented as a short Python script that uses the prototype compiler’s implementation of the `ModelNeighbors` algorithm described in section 6.3. Its source code is available online [20].

Starting from the case study’s first model, the greedy graph search followed the path shown in fig. 10:

The search performed 47 ELPD evaluations. The search agreed with the case study authors’ final model, confirming that it has (at least locally) optimal predictive performance.

While greedy maximization of ELPD is a naive statistical workflow and shouldn’t be blindly trusted it to give a final model, it is at least useful for finding promising neighborhoods, especially for large model spaces.

10 Future work

As discussed in section 1.1, there are many motivating use cases for the network of models. We hope to demonstrate and build tooling for more of these use cases, using modular Stan as a foundation:

- Model search. Section 9.3 gave a simple algorithm for greedy search that only used the network topology. We hypothesize that more efficient search methods could leverage the module structure, treat search as an exploration/exploitation problem, or utilize methods from the symbolic regression literature.

- Model space navigation tools. Model developers must decipher promising directions in which to iterate. If we could annotate the edges be-
Figure 10: The red annotations show the ELPD scores for the assessed models. The search algorithm visited nodes along the red arrow path from starting at [START] and terminating at [GOAL].
tween models with meaningful joint metrics, we could provide developers with direction. We could also use model statistics or edge weights to embed network-space into visualizations.

- Multi-model ensemble methods. As mentioned in section 1.1, multi-model ensemble methods like stacking and multiverse analysis could be applied to multi-model programs.

- Sensitivity analysis. To automate sensitivity analysis given a model and some metric of a model’s results, like a \( p \)-value, we can check the extent to which the model’s results differ from its neighbors.

In addition, we hope to expand the capabilities of the swappable module system.

- Explicit model signatures. Thought we believe that our module signature inference scheme is more beginner-friendly, explicit signatures would make module reuse across applications easier.

- Implementation co-selection logic. While features like module fields allow users to encode the constraint that a set of implementations should always be selected together, there is no reason that user constraints on selection sets should not be arbitrarily complex, the end point being a predicate logic.
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