Making Better Choices

Guiding Random Generators with Derivatives

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Abstract

When generating random data structures, it is often important that the generated values are in some way *valid*. This is especially important in areas like property-based testing, where test inputs are only useful if they satisfy a property's precondition. We tackle this "valid generation problem" by observing that, perhaps surprisingly, random *generators* are closely related to *parsers*. In particular, both generators and parsers make a sequence of choices that are used build a data structure piece by piece.

This insight leads us to a rich theory of *free generators* that makes the connection between generators and parsers explicit; free generators can be interpreted as either generators or parsers as needed and can be manipulated syntactically. In particular, free generators admit an efficiently computable notion of *derivative* that can be used to preview the effect of a particular choice in the generator. We use this derivative operation in a novel algorithm that aims to solve the problem of generating valid data structures in certain domains.

Keywords: Property-based testing, Formal languages, Random generation

1 Introduction

Various uses for random data structures are subject to the *valid generation problem*—they need a large number of the random values that satisfy some validity condition. For our purposes, we specifically care about black-box, computable validity predicates. For example, we may want to generate random binary trees such that they are valid binary *search* trees (BSTs) according to an isBST function. The challenge is to randomly generate a variety of valid data structures as quickly as possible.

This problem is especially common when using tools like QuickCheck [4] for *property-based testing*. Property-based testing checks that a program obeys a functional specification using hundreds or thousands of random inputs. Testers run into the valid generation problem when their specifications have preconditions. For example, in order to test that an insert procedure preserves the BST invariants, one needs to generate lots of inputs that are already BSTs. A naïve generator might produce relatively few valid inputs in a given period of time, so testers often resort to bespoke generation algorithms, but ideally the necessary inputs could be produced more automatically.

The valid generation problem is computationally hard in general, but various approaches have shown promise [3, 6, 11]. We choose to focus on *generator optimization*, which is an active area of research [15, 16]. These methods start with an existing generator (which does not produce exclusively valid values) and tune or modify the generator to produce valid results with higher-than-normal probability. In particular, our work explores new avenues for generator optimization that hinge on a simple observation: generators operate like *parsers* of random choices.

What exactly does it mean for a generator to act like a parser? A random generator is a program that makes a sequence of random choices—essentially coin-flips—to decide how some value should be constructed. As the program runs, each choice is made in real-time by calling `rand()` or another similar function. Of course, there is nothing stopping us from pre-computing choices for the generator to use; we could provide a list of choices ahead of time and tell the generator to make those choices one after the other. This mode of operation is exactly parsing!

We make this intuition concrete with objects that we call *free generators*, which re-imagine standard random generators as syntax trees that can be interpreted and manipulated at will. Free generators can be viewed as normal generators, which make real-time choices, but they can also be interpreted as deterministic parsers of sequences of choices in the way we observed above. This gives a concrete understanding of the close connection between generation and parsing, clarifying existing folklore into a useful formalism.

Free generators are inspired by *Free Applicative Functors* [2], and accordingly, they are incredibly flexible. They are not tied to a particular output distribution, so we can modify the average size and shape of output values without modifying the actual generator. But changing the distribution does not yet give us a way to solve the valid generation problem. For that, we rely on the fact that free generators are represented as data structures that can be manipulated by programs.

We can define a *derivative* operation on free generators that computes a new generator representing the same generator with the first choice already fixed. In the case of our binary search tree example, this might fix a particular value for a

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node, or fix a stopping point for a particular sub-tree. We can use derivatives to evaluate how likely a given choice is to produce valid results. This yields a new approach to the valid generation problem that has done remarkably well in our experiments.

In the next section, we describe the high-level motivation behind our free generator formalism and give an overview of potential applications that justify the theory in the remainder of the paper (§2). After that, we make the following contributions:

- We present a novel theory of *free generators* that gives a formal account of the connections between random generators and parsers (§3).
- We define a *derivative* operation on free generators that computes a view of a generator after making a particular choice and prove this operation consistent with related notions in formal languages (§4).
- We give an algorithm for tackling the *valid generation problem* that relies on free generator derivatives (§5).

We conclude with related work (§6) and ideas for future research (§7).

2 The High-Level Story

This section gives a bird's-eye view of our motivation, theory, and exploratory evaluation.

2.1 Generators and Parsers

The goal of this work is to optimize an existing generator by observing that generators are like parsers. Let us start by looking at a specific generator and understanding what it has in common with a specific parser.

Consider genTree, defined in Figure 1. The program genTree is a generator that produces random binary trees of Booleans like

Node True Leaf Leaf and
Node True Leaf (Node False Leaf Leaf)

by making a series of random choices (represented here as uniform coin flips). The choices lead the program to generate trees up to a given height via a simple recursive procedure. Note that the generator does not always make the same number of choices: sometimes it chooses to return a Leaf and terminate, and other times it chooses to build a Node, which requires more choices.[1]

Now, consider parseTree (also in Figure 1), which parses a tree from a string containing the characters `n`, `l`, `t`, and `f`. The parser turns

`ntll` into Node True Leaf Leaf and
`ntlnfll` into Node True Leaf (Node False Leaf Leaf).

[1]One might wonder why we do not simply produce trees like this from a CFG or PCFG: in this case we could, but in general expressing generators as programs like this is more powerful and flexible. Specifically, the generator languages we work with can make sequences of choices with context-sensitive structure.

```
genTree h =
  if h = 0 then
    return Leaf
  else
    c ← flip()
    if c == Head then return Leaf
    if c == Tail then
      c ← flip()
      if c == Head then x ← True
      if c == Tail then x ← False
      l ← genTree (h − 1)
      r ← genTree (h − 1)
      return Node x l r

parseTree h =
  if h = 0 then
    return Leaf
  else
    c ← consume()
    if c == 'l' then return Leaf
    if c == 'n' then
      c ← consume()
      if c == 't' then x ← True
      if c == 'f' then x ← False
      else fail
      l ← parseTree (h − 1)
      r ← parseTree (h − 1)
      return Node x l r
    else fail
```

Figure 1. A generator and a parser for Boolean binary trees.

The parser operates character by character, sometimes changing the way it handles the next character based on the previous character.

At this point the superficial similarities between genTree and parseTree should be clear, but what is really going on? It all comes down to *choices*. In genTree, choices are made randomly during the execution of the program, while in parseTree the choices were made ahead of time and manifest as the characters in the input string. The programs have the same structure, and only differ in their expectation of when choices should be made. Ideally, we should always be able to re-interpret a generator as a parser of sequences of choices, or a parser as a generator over its output set.

2.2 Free Generators

We can unify random generation with parsing by abstracting both ideas into a single data structure. For this, we introduce free generators.[2] Free generators are not traditional programs

[2]This document uses the `knowledge` package in LaTeX to make definitions interactive. Readers viewing the PDF electronically can click on technical terms and symbols to see where they are defined in the document.

like genTree or parseTree, they are more like abstract syntax trees. Taking inspiration from *Free Applicative Functors* [2], free generators are data structures that can be *interpreted* as programs with a similar shape.

```
fgenTree h =
  if h = 0 then
    Pure Leaf
  else
    Select
      [ (l, Pure Leaf),
        (n, MapR
          (Pair (Select
                  [ (t, Pure True),
                    (f, Pure False) ])
                (Pair (fgenTree (h - 1))
                      (fgenTree (h - 1))))
          (λ (x, (l, r)) → Node x l r)) ]
```

Figure 2. A free generator for Boolean binary trees.

In §3 we give a domain-specific language for constructing free generators that is almost identical to the normal way users would construct generators with QuickCheck. But we give an example here that is explicitly built from data constructors order to make it clear that these are data structures, not normal programs.

This makes everything a bit harder to interpret, but the details are not critical; instead, look at Figure 2 and notice the structural similarities between that free generator and the examples in Figure 1.

We can use fgenTree to construct a free generator for Boolean binary trees of a given height. When reading the data structure, think of Pure in almost the same way as **return** from the previous examples, returning a pure value without making any choices or parsing any characters. MapR takes two arguments, a free generator and a function that can be applied to the result that is generated/parsed. (In §3 we define Map instead, which is the same, but the arguments are reversed.) The Pair constructor does a sort of sequencing: it generates/parses using its first argument, then it does the same with its second argument, and finally it pairs the results together. Finally, the real magic is in the way we interpret the Select structure. When we want a generator, we treat it as making a uniform random choice, and when we want a parser we treat it as consuming a character and checking c against the first elements of the pairs.

The almost line-to-line correspondence between fgenTree and genTree (or parseTree) is no accident! In §3 we give formal definitions of free generators, along with a number of interpretation functions. We use $\mathcal{G}[\![\cdot]\!]$ to mean the generator interpretation of a free generator and $\mathcal{P}[\![\cdot]\!]$ to mean the parser interpretation of a free generator. In other words,

$$\mathcal{G}[\![\text{fgenTree } 5]\!] \approx \text{genTree } 5 \quad \text{and}$$
$$\mathcal{P}[\![\text{fgenTree } 5]\!] \approx \text{parseTree } 5.$$

These functions mean that we can write one free generator that can be used in different ways depending on what we need at the moment.

We also define $C[\![g]\!]$ to be the choice distribution of a free generator. Intuitively, the choice distribution should produce the sequences of choices that the generator interpretation can make, or equivalently the sequences that the parser interpretation can parse. To make this relationship formal, we prove Theorem 3.4, which says that for any free generator g,

$$\mathcal{P}[\![g]\!] \langle\$\rangle\, C[\![g]\!] \approx \mathcal{G}[\![g]\!]$$

(where $\langle\$\rangle$ is defined as a kind of "mapping" operation over distributions). Another way to read this theorem is that generators can be factored into two pieces: a distribution over choice sequences (given by $C[\![\cdot]\!]$), and a parser of those sequences (given by $\mathcal{P}[\![\cdot]\!]$).

We can work with those pieces independently if we wish. For example, we can replace $C[\![g]\!]$ with some other distribution over choice sequences to obtain a generator with a totally different output distribution but the same overall structure.

Besides swapping out a generator's distribution, there are other reasons to prefer a free generator to a normal generator. In the next section, we see how free generators can be syntactically manipulated.

2.3 Derivatives of Free Generators

Every parser defines a formal language of the strings that it can successfully parse. Similarly, we define the language interpretation of a free generator $\mathcal{L}[\![g]\!]$ to be the set of choice sequences parsed (or made) by the generator. Viewing free generators this way suggests some interesting ways that free generators might be manipulated.

Formal languages have a notion of *derivative* that is attributed to Brzozowski [1]. For a formal language L, the Brzozowski derivative is defined as:

$$\delta_c L = \{s \mid c \cdot s \in L\}$$

In other words, the derivative of L with respect to c is all strings in L that start with c, with the first c removed.

Some models of languages, including regular expressions and context-free grammars, allow syntactic transformations that correspond to derivatives. While parser programs like parseTree cannot literally be modified in this way, we can still imagine what such a transformation would look like. Conceptually, the derivative of a parser with respect to a character c is whatever parser remains assuming c has just been parsed.

For example, if we fix height = 5 for simplicity, we can think of the derivative of parseTree 5 with respect to n as:

```
δn(parseTree 5) ≈
    c ← consume()
    if c == t then x ← True
    if c == f then x ← False
    else fail
    l ← parseTree 4
    r ← parseTree 4
    return Node x l r
```

This parser is "one step" simpler than parseTree. After parsing the character n, the next step is to parse either t or f and then construct a Node, so the derivative does just that.

We can imagine another step and look at the derivative of δ_n(parseTree 5) with respect to t:

```
δt δn(parseTree 5) ≈
    l ← parseTree 4
    r ← parseTree 4
    return Node True l r
```

Now we have fixed the value True for x, and we can continue by making the recursive calls and constructing the final tree.

Our free generators also have a closely related notion of derivative! We can take derivatives of the free generator produced by fgenTree that look almost identical to the ones that we saw for parseTree:

```
δn(fgenTree 5) ≈
    MapR
      (Pair (Select
              [ (t, Pure True),
                (f, Pure False) ])
            (Pair (fgenTree 4)
                  (fgenTree 4)))
      (λ (x, (l, r)) → Node x l r)
```

and

```
δt δn(fgenTree 5) ≈
    MapR
      (Pair (fgenTree 4)
            (fgenTree 4))
      (λ (l, r) → Node True l r)
```

These derivatives are also easy to compute. In §4 we define a simple procedure for computing the derivative of a free generator and show that the definition behaves the way we want. Formally, we prove Theorem 4.2 which says:

$$\delta_c \mathcal{L}[\![g]\!] = \mathcal{L}[\![\delta_c g]\!].$$

In other words, the derivative of the language of a generator g is equal to the language of the derivative of g.

We can think of the derivative of a free generator as the generator that remains after parsing *or making* a choice. This means that we can essentially preview the result of making a choice without actually interpreting the generator. In the next section, we show the practical applications of this technique.

2.4 The Choice Gradient Sampling Algorithm

This section introduces Choice Gradient Sampling (CGS), an algorithm for generating data that satisfies a validity condition. Given a simple free generator, CGS builds on the ideas in the previous section: it previews choices using derivatives. In fact, it previews all possible choices, essentially taking the *gradient* of the free generator. For example,

$$\nabla g = \{\delta_a g,\ \delta_c g,\ \delta_c g\}$$

Each derivative in the gradient can be sampled to get a sense of how good or bad the respective choice was. This provides a metric that guides the algorithm to valid inputs.

An example execution of CGS shown pictorially in Figure 3. Starting from g we take the gradient of g by taking the derivative with respect to each possible character, in this case a, b, and c. Then we evaluate each of the derivatives by (1) interpreting the generator with $\mathcal{G}[\![\cdot]\!]$, (2) sampling values from the resulting generator, and (3) counting how many of those results are valid with respect to φ. The result of (3) is values f_a, f_b, and f_c, which we can think of as relative weights for how likely each choice is to lead us to a valid result. We then pick a choice randomly, weighted based on the values for f, and continue until our choices produce an output.

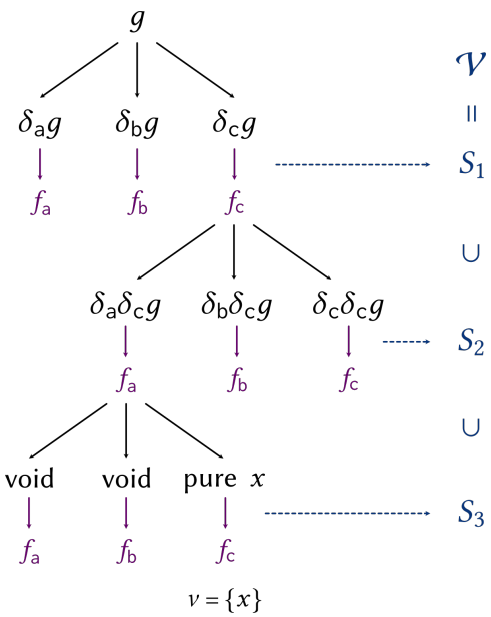

Figure 3. Choice Gradient Sampling: Generating valid values, $\mathcal{V}$, with free generator derivatives.

Critically, we avoid wasting effort by saving the samples (S_1, S_2, S_3, etc.) that we use to evaluate the gradients. Many of those samples will be valid results that we can use, so there is no reason to throw them away. The final result $\mathcal{V}$ is the union of all of the valid samples, plus the final valid result (called x in the diagram). There are more algorithmic details that we elide until §5.

2.5 Exploratory Evaluation

To validate the efficacy of Choice Gradient Sampling, we evaluate it on benchmarks that are often found in the property-based testing literature. Specifically, we compare CGS to the default way QuickCheck handles properties with preconditions (assuming there is no bespoke generator available), rejection sampling. We chose rejection sampling, rather than more state-of-the-art comparisons [3, 16], because our primary goal was to validate our theory, not to produce a production-ready tool.

Our high-level results are given in Table 1, which shows the total number of unique, valid values that each algorithm (CGS and Rejection) generates in the span of 60 seconds. These numbers are quite promising—CGS is always able to generate more unique values than Rejection in the same amount of time, and it often generates *significantly* more.

	BST	SORTED	AVL	STLC
Rejection	9,762	6,452	156	106,282
CGS	22,286	59,436	221	298,001

Table 1. Unique valid values generated in 60 seconds.

We provide the details of all of our benchmarks in §5 (the experimental parameters are given in Table 2), but for now we focus on just one benchmark: **STLC**. Our **STLC** benchmark evaluates how well CGS can generate well-typed terms of a simply-typed lambda calculus.

We write an extremely simple free generator called fgenExpr that generates lambda-terms with no thought given to types; we intend for such a generator to be straightforwardly synthesized from type information alone. We then pass fgenExpr (along with a sample-rate constant of $N = 400$) to CGS and allow it to generate well-typed lambda terms for one minute. Again, total number of unique terms generated is shown in Table 1, but unique terms alone does not tell the whole story.

The plots in Figure 4 give some deeper insights. The first plot ("Unique Terms over Time") shows that after one minute, CGS has not yet "run out" of unique terms to generate. The "Normalized Size Distribution" chart shows that CGS also generates larger terms on average. This is great from the perspective of property-based testing, where test size is often positively correlated with bug-finding power since larger test inputs tend to exercise more of the implementation code. Finally, "Normalized Constructor Frequency" demonstrates some room for improvement: the higher green bars for "Plus" and "Lit*n*" suggest that CGS capitalizes on the fact that integer expressions are easy to generate by slightly biasing generation towards terms containing them. However, this effect is minor, and **STLC** is actually our worst-performing benchmark in that regard.

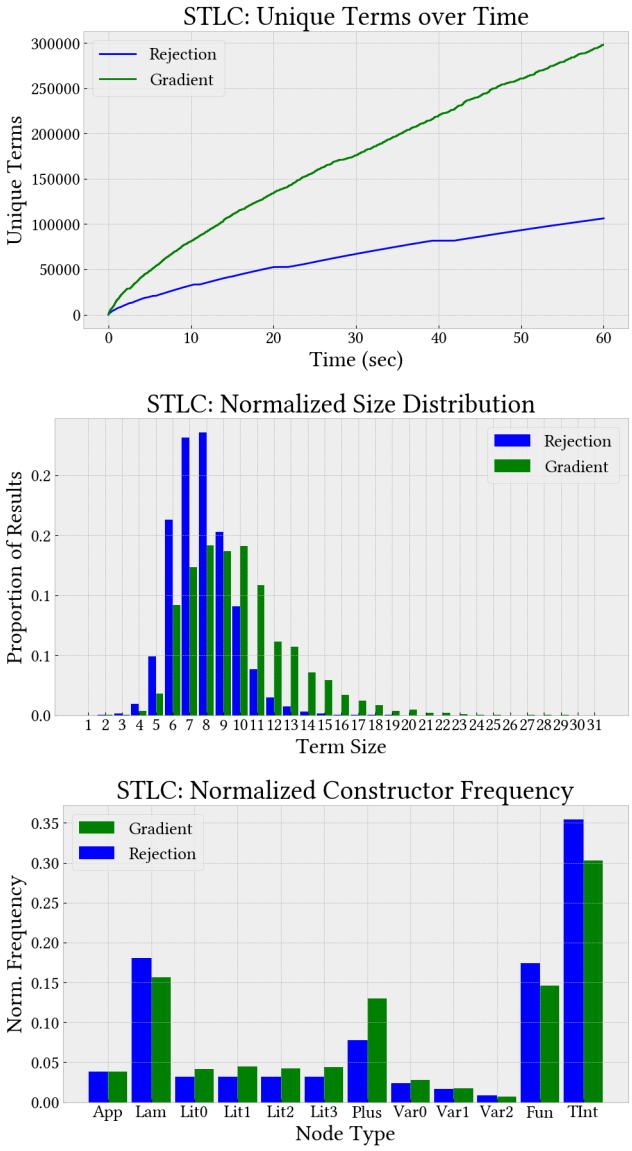

Figure 4. Unique values and term sizes for the **STLC** benchmark.

Overall we are quite happy with these results. We have demonstrated that Choice Gradient Sampling is able to generate valid values for structures with complex preconditions, and that it generates values that are larger than the values generated via rejection sampling. Again, §5 has more detail, including analysis of random value diversity and explanation of the relatively poor performance of **AVL**.

3 Free Generators in Detail

In this section, we develop the theory of *free generators*. We start with some background information on applicative abstractions for parsing and random generation and then present our new framing of generators that makes choices explicit and enables interesting syntactic manipulations.

3.1 Background: Applicative Parsers and Generators

In §2 we represent generators and parsers with pseudo-code. Here we bridge the gap between the code in that section and the code that users of our theory would actually work with.

We represent both generators and parsers using *applicative functors* [14]. At a high level, an applicative functor as a type constructor f with an operation,

```
(⟨$⟩) :: (a → b) → f a → f b
```

also known as "fmap" and operations,

```
pure :: a → f a
(⟨*⟩) :: f (a → b) → f a → f b
```

the latter of which is often called "TIE". At first these operations may seem fairly esoteric, but they really just define a convenient way to apply functions underneath the type constructor f structure. For example, the idiom `g ⟨$⟩ x ⟨*⟩ y ⟨*⟩ z` applies a pure function g to three structures x, y, and z.

We can use these operations to define genTree like we would in QuickCheck [4], since the type constructor Gen representing generators is an applicative functor:

```
genTree :: Int → Gen Tree
genTree 0 = pure Leaf
genTree h =
  oneof [ pure Leaf,
          Node ⟨$⟩ genInt
               ⟨*⟩ genTree (h - 1)
               ⟨*⟩ genTree (h - 1) ]
```

In this context, pure is the trivial generator that always generates the same value, and `Node ⟨$⟩ g1 ⟨*⟩ g2 ⟨*⟩ g3` means apply the constructor Node under three sub-generators to produce a new generator. (Operationally, this means sampling x1 from g1, x2 from g2, and x3 from g3, and then constructing Node x1 x2 x3.) Notice that we need one extra function beyond the applicative interface: oneof makes a uniform choice between generators, just as we saw in the pseudo-code.

We can do the same thing for parseTree, using combinators inspired by *Parsec* [12] (this time because Parser is applicative):

```
parseTree :: Int → Parser Tree
parseTree 0 = pure Leaf
parseTree h =
  choice [ (1, pure Leaf),
           (n, Node ⟨$⟩ parseInt
                    ⟨*⟩ parseTree (h - 1)
                    ⟨*⟩ parseTree (h - 1)) ]
```

In this context, pure is a parser that consumes no characters and never fails, it just produces the value passed to it. We can interpret `Node ⟨$⟩ p1 ⟨*⟩ p2 ⟨*⟩ p3` as running each sub-parser in sequence (failing if any of them fail) and then wrapping the results in the Node constructor. Finally, we have replaced oneof with choice, but the idea is the same: choose between sub-parsers.[3]

Parsers of this form have type `String → Maybe (a, String)`. They can be applied to a string to obtain either Nothing or `Just (a, s)`, where a is the parse result and s contains any extra characters.

3.2 Representing Generators

With the applicative interface in mind, we can now give the formal definition of a *free generator*.[4]

3.2.1 Type Definition.

We represent free generators as an inductive data type, FGen, defined as:

```
data FGen a where
  Void :: FGen a
  Pure :: a → FGen a
  Pair :: FGen a → FGen b → FGen (a, b)
  Map :: (a → b) → FGen a → FGen b
  Select :: [(Char, FGen a)] → FGen a
```

These constructors form a sort of abstract syntax tree with constructors that each correspond to some function from the interfaces in the previous section. Clearly Pure represents pure. Pair is a slightly different form of ⟨*⟩—one is definable from the other, but this version makes more sense as a data constructor. Map corresponds to ⟨$⟩. Finally, Select subsumes both oneof and choice—it might mean either, depending on the interpretation.

Recall that free generators are inspired by free applicative functors. This means that we can write a transformation from `FGen a → f a` for any f with similar structure. This fact motivates the rest of this section.

3.2.2 Language of a Free Generator.

We say that the *language of a free generator* is the set of choice sequences that it might make or parse. We define a generator's language recursively, by cases:

$$
\begin{aligned}
&\mathcal{L}[\![\cdot]\!] :: \mathsf{FGen\ a} \to \mathsf{Set\ \ String} \\
&\mathcal{L}[\![\mathsf{Void}]\!] &&= \emptyset \\
&\mathcal{L}[\![\mathsf{Pure\ a}]\!] &&= \varepsilon \\
&\mathcal{L}[\![\mathsf{Map\ f\ x}]\!] &&= \mathcal{L}[\![\mathsf{x}]\!] \\
&\mathcal{L}[\![\mathsf{Pair\ x\ y}]\!] &&= \{\mathsf{s} \cdot \mathsf{t} \mid \mathsf{s} \in \mathcal{L}[\![\mathsf{x}]\!] \wedge \mathsf{t} \in \mathcal{L}[\![\mathsf{y}]\!]\} \\
&\mathcal{L}[\![\mathsf{Select\ xs}]\!] &&= \{\mathsf{c} \cdot \mathsf{s} \mid (\mathsf{c}, \mathsf{x}) \in \mathsf{xs} \wedge \mathsf{s} \in \mathcal{L}[\![\mathsf{x}]\!]\}
\end{aligned}
$$

[3] For clarity, we have slightly modified the interface for applicative parsers; *Parsec* has different way of expressing choice.

[4] For algebraists: free generators are "free," in the sense that they admit unique structure-preserving maps to other "generator-like" structures. In particular, the $\mathcal{G}[\![\cdot]\!]$ and $\mathcal{P}[\![\cdot]\!]$ maps are canonical. For the sake of space, we do not explore these ideas rigorously.

3.2.3 Smart Constructors and Simplified Forms.

Free generators admit a useful *simplified form*. We ensure that generators are simplified by requiring that free generators are built with *smart constructors*.

Instead of Pair, users should pair free generators with ⊗:

```
(⊗) :: FGen a → FGen b → FGen (a, b)
Void    ⊗ _       = Void
_       ⊗ Void    = Void
Pure a  ⊗ y       = (λb → (a, b)) ⟨$⟩ y
x       ⊗ Pure b  = (λa → (a, b)) ⟨$⟩ x
x       ⊗ y       = Pair x y
```

which makes sure that Void and Pure are simplified as much as possible with respect to Pair. Next, ⟨$⟩ is a version of Map that does similar simplifications:

```
(⟨$⟩) :: (a → b) → FGen a → FGen b
f ⟨$⟩ Void    = Void
f ⟨$⟩ Pure a  = Pure (f a)
f ⟨$⟩ x       = Map f x
```

We define pure and ⟨∗⟩ to make FGen an applicative functor:

```
pure :: a → FGen a
pure = Pure
(⟨∗⟩) :: FGen (a → b) → FGen a → FGen b
f ⟨∗⟩ x = (λ (f, x) → f x) ⟨$⟩ (f ⊗ x)
```

Finally, we define a smart constructor for Select:

```
select :: [(Char, FGen a)] → FGen a
select xs =
  case filter (λ (_, p) → p ≠ Void) xs of
    [] → ⊥
    xs | duplicates (map (λ (c, _) → c) xs) → ⊥
    xs → Select xs
```

Unlike the other smart constructors, select can fail. This helps us ensure that generators make sense later on—for example, our interpretation of choices means that it is not clear what it would mean the same choice label to appear twice in a given call to Select. When generators are built with only smart constructors, we say they are in simplified form.

3.2.4 Examples.

As one would hope, we can generalize our definitions from earlier in this section to get a single free generator fgenTree that subsumes genTree and parseTree.

```
fgenTree :: Int → FGen Tree
fgenTree 0 = pure Leaf
fgenTree h =
  select [ (1, pure Leaf),
           (n, Node ⟨$⟩ fgenInt
                    ⟨∗⟩ fgenTree (h - 1)
                    ⟨∗⟩ fgenTree (h - 1)) ]
```

Excitingly, even though we are building a data structure we can write it like a program with exactly the same abstractions that are used for constructing generators and parsers.

Another good example of a free generator fgenExpr, which is used in our **STLC** benchmark to produce random terms of a simply-typed lambda-calculus:

```
data Type = TInt | TFun Type Type
data Expr
  = Lit Int | Plus Expr Expr
  | Lam Type Expr | Var Int | App Expr Expr

fgenExpr :: Int → FGen Expr
fgenExpr 0 =
  select [ (i, Lit ⟨$⟩ fgenInt),
           (v, Var ⟨$⟩ fgenVar) ]
fgenExpr h =
  select [ (i, Lit ⟨$⟩ fgenInt),
           (p, Plus ⟨$⟩ fgenExpr (h - 1)
                    ⟨∗⟩ fgenExpr (h - 1)),
           (l, Lam ⟨$⟩ fgenType
                   ⟨∗⟩ fgenExpr (h - 1)),
           (a, App ⟨$⟩ fgenExpr (h - 1)
                   ⟨∗⟩ fgenExpr (h - 1)),
           (v, Var ⟨$⟩ fgenVar) ]
```

Structurally this is very similar to the previous generator, it just has more cases and more choices. Our lambda calculus is constructed with de Bruijn indices for variables and has integers and functions as values. The language is exceedingly simple, but generating well-typed terms is still fairly difficult. Thus we consider this example a useful case study.

Remark. One might be concerned that these free generators are quite large, growing exponentially in h. We are able to avoid most size-related issues in Haskell due to laziness—the parts of the structure that are not yet needed are left uninterpreted—but we recognize that relying on laziness is a bit unsatisfying. Luckily it would be straightforward to share the recursive calls to fgenExpr (h - 1) between all of the branches of the Select node (and the Pairs below that) and avoid any blowup. This is simple in languages with pointers, and it side-steps the exponential growth entirely. A similar approach could be taken in pure functional languages like Haskell, although it would require more complex data structures that would obscure the important parts of our presentation.

3.3 Interpreting Free Generators

A free generator does not *do* anything on its own—it is simply a data structure. In this section, we see the formal definitions of the interpretation functions that we discussed in §2 and prove a theorem that links those interpretations together.

3.3.1 As a Generator of Values.

The most natural way to interpret a free generator is as a QuickCheck generator—that is, as a distribution over some data structure. We define the *generator interpretation* of a free generator to be:

```
𝒢⟦·⟧ :: FGen a → Gen a
𝒢⟦Void⟧       = ⊥
𝒢⟦Pure v⟧     = pure v
𝒢⟦Map f x⟧    = f ⟨$⟩ 𝒢⟦x⟧
𝒢⟦Pair x y⟧   =
  (λx y → (x, y)) ⟨$⟩ 𝒢⟦x⟧ ⟨*⟩ 𝒢⟦y⟧
𝒢⟦Select xs⟧  =
  oneof (map (λ (_, x) → 𝒢⟦x⟧) xs)
```

One detail worth noting is that the interpretation behaves poorly on Void, but we can prove a lemma to show that this does not cause problems in practice:

Lemma 3.1. *If a generator g is simplified,*

$$g = \mathit{Void} \iff g \text{ contains } \mathit{Void}.$$

Proof. By induction on the structure of g and inspection of the smart constructors. □

Thus we can conclude that as long as g is in simplified form and not Void, $\mathcal{G}[\![g]\!]$ is defined.

Example 3.2. As desired, $\mathcal{G}[\![$fgenTree 5$]\!]$ is equivalent to genTree 5.

3.3.2 As Parser of Choice Sequences.

Of course, there would be no point in defining free generators if we were only going to interpret them as QuickCheck generators. We can make use of the choice labels using the free generator's *parser interpretation*—in other words, viewing it as a parser of choices as we originally wanted. The translation looks like:

```
𝒫⟦·⟧ :: FGen a → Parser a
𝒫⟦Void⟧       = λs → Nothing
𝒫⟦Pure a⟧     = pure a
𝒫⟦Map f x⟧    = f ⟨$⟩ 𝒫⟦x⟧
𝒫⟦Pair x y⟧   =
  (λx y → (x, y)) ⟨$⟩ 𝒫⟦x⟧ ⟨*⟩ 𝒫⟦y⟧
𝒫⟦Select xs⟧  =
  choice (map (λ (c, x) → (c, 𝒫⟦x⟧)) xs)
```

This definition uses the representation of parsers as functions of type String → Maybe (a, String) that we saw earlier. Error handling happens under the hood for operations like Pair.

Example 3.3. As desired, $\mathcal{P}[\![$fgenTree 5$]\!]$ is equivalent to parseTree 5.

3.3.3 As a Generator of Choice Sequences.

Our final interpretation of free generators is a sort of dual to the previous one. Instead of throwing away randomness in favor of deterministic parsing, we can extract only the random distribution and ignore everything about how result values are constructed. We define the *choice distribution* of a free generator to be:

```
C⟦·⟧ :: FGen a → Gen String
C⟦Void⟧       = ⊥
C⟦Pure a⟧     = pure ε
C⟦Map f x⟧    = C⟦x⟧
C⟦Pair x y⟧   =
  (λs t → s · t) ⟨$⟩ C⟦x⟧ ⟨*⟩ C⟦y⟧
C⟦Select xs⟧  =
  oneof (map (λ (c, x) → (λs → c · s) ⟨$⟩ C⟦x⟧) xs)
```

Note that we can equivalently think of this as a distribution over $\mathcal{L}[\![g]\!]$.

3.3.4 Coherence.

We would like for our three interpretations of free generators to make sense together. We call this property coherence, and prove it in this section.

We say two generators are *equivalent*, written $g_1 \equiv g_2$, if and only if the generators represent the same distribution over values. Any equal generators are trivially equivalent, but for technical reasons, properties concerning ⟨$⟩, ⟨*⟩, etc. are generally only valid up to this notion of equivalence. With this in mind, we can state our coherence theorem and sketch the proof:

Theorem 3.4 (Factoring Coherence)**.** *Every simplified free generator can be factored coherently into a parser and a distribution over choice sequences. In other words, for all simplified free generators $g \neq \mathit{Void}$,*

$$\mathcal{P}[\![g]\!] \langle\$\rangle\, C[\![g]\!] \equiv (\lambda x \to \mathit{Just}\ (x, \varepsilon)) \langle\$\rangle\, \mathcal{G}[\![g]\!].$$

Proof sketch. We proceed by induction on the structure of g.

Case g = Pure a. Straightforward.

Case g = Map f x. Straightforward.

Case g = Pair x y. This case is the most interesting one. The difficulty is that it is not immediately obvious why

$$\mathcal{P}[\![\text{Pair x y}]\!] \langle\$\rangle\, C[\![\text{Pair x y}]\!]$$

should be a function of

$$\mathcal{P}[\![\text{x}]\!] \langle\$\rangle\, C[\![\text{x}]\!] \quad \text{and} \quad \mathcal{P}[\![\text{y}]\!] \langle\$\rangle\, C[\![\text{y}]\!].$$

Showing the correct relationship requires a lemma that says that for any sequence s generated by $C[\![$x$]\!]$ and an arbitrary sequence t, there is some a such that

$$\mathcal{P}[\![\text{x}]\!]\ (s \cdot t) = \text{Just}\ (a, t).$$

Case g = Select xs. The reasoning in this case is a bit subtle, since it requires certain operations to commute with Select, but the details are not particularly instructive.

See Appendix B for the full proof. □

3.4 Replacing a Generator's Distribution

Since a generator g can be factored using $C[\![\cdot]\!]$ and $\mathcal{P}[\![\cdot]\!]$, we can explore what it would look like to modify a generator's distribution (i.e., change or replace $C[\![\cdot]\!]$) without having to modify the entire generator.

Suppose we have some other distribution that we want our choices to follow, represented as a function from a history of choices to a generator of next characters:

```
type DistF = String → Gen (Maybe Char)
```

(If the next choice is Nothing, then generation stops.) We can be a bit more general and pair a distribution function with a "current" history, to get our formal definition of a custom choice distribution:

```
type Dist = (String, DistF)
```

A Dist may be arbitrarily complex—in particular, it might contain information obtained from a machine learning model, example-based tuning, or some other automated tuning process. How would we use such a distribution in place of the standard distribution given by $C[\![\cdot]\!]$?

The solution is actually quite elegant: we just replace $C[\![\cdot]\!]$ with a distribution to yield the *definition*:

```
G[[·]] :: (Dist, FGen a) → Gen (Maybe a)
G[[((h, d), g)]] = P[[g]] ⟨$⟩ genDist h
  where
    genDist h = d h >>= λx → case x of
      Nothing → pure h
      Just c → genDist (h · c)
```

Whereas before we proved an equivalence between $\mathcal{G}[\![g]\!]$ and $\mathcal{P}[\![g]\!]\langle\$\rangle\ C[\![g]\!]$, we can now use that relationship as a definition of what it means to interpret a generator under a new distribution.

Since replacing a free generator's distribution does not actually change the structure of the generator, we can have a different distribution for each use-case of the free generator. In a property-based testing scenario, this might mean a finely-tuned distribution for each property, carefully optimized to find bugs as quickly as possible.

4 Derivatives of Free Generators

So far we have presented free generators and shown that they can be interpreted in a number of useful ways. In this section, we review the notion of Brzozowski derivative in formal language theory and we show that a similar operation exists for free generators.

4.1 Background: Derivatives of Languages

The *Brzozowski derivative* [1] of a formal language L with respect to some character c is defined as

$$\delta_c L = \{s \mid c \cdot s \in L\}.$$

In other words, the derivative is the set of strings in L with c removed from the front. For example,

$$\delta_{\mathsf{a}}\{\mathsf{abc}, \mathsf{aaa}, \mathsf{bba}\} = \{\mathsf{bc}, \mathsf{aa}\}.$$

Many language representations have syntactic transformations that correspond to Brzozowski derivatives. For example, we can take the derivative of a regular expression in the following way:

$$\begin{aligned}
\delta_c \varnothing &= \varnothing \\
\delta_c \varepsilon &= \varnothing \\
\delta_c \mathsf{c} &= \varepsilon \quad (c = \mathsf{c}) \\
\delta_c \mathsf{d} &= \varnothing \quad (c \neq \mathsf{d}) \\
\delta_c(r_1 + r_2) &= \delta_c r_1 + \delta_c r_2 \\
\delta_c(r_1 \cdot r_2) &= \delta_c r_1 \cdot r_2 + \nu r_1 \cdot \delta_c r_2 \\
\delta_c(r^*) &= \delta_c r \cdot r^*
\end{aligned}
\qquad
\begin{aligned}
\nu\varnothing &= \varnothing \\
\nu\varepsilon &= \varepsilon \\
\nu\mathsf{c} &= \varnothing \\
\nu(r_1 + r_2) &= \nu r_1 + \nu r_2 \\
\nu(r_1 \cdot r_2) &= \nu r_1 \cdot \nu r_2 \\
\nu(r^*) &= \varepsilon
\end{aligned}$$

The ν operator, used in the "$\cdot$" rule, determines the *nullability* of an expression (whether or not it accepts ε). As one would hope, if r has language L, it is always the case that $\delta_c r$ has language $\delta_c L$.

4.2 The Free Generator Derivative

Since free generators define a language (given by $\mathcal{L}[\![\cdot]\!]$), it makes sense to ask: can we take their derivatives? Yes! We define the *derivative of a free generator* to be:

```
δ :: Char → FGen a → FGen a
δc Void        = Void
δc (Pure v)    = Void
δc (Map f x)   = f ⟨$⟩ δc x
δc (Pair x y)  = δc x ⊗ y
δc (Select xs) = if (c, x) ∈ xs then x else Void
```

These definitions should be mostly intuitive. The derivative of a generator that does not make a choice (i.e., Void and Pure) is Void, since the corresponding language would be empty. Map does not affect the derivative, since it is concerned with choices, not the final result. The derivative of Select is just the argument generator corresponding to the appropriate choice.

The one potentially confusing case is the one for Pair. We have defined the derivative of a pair of generators by taking the derivative of the first generator in the pair and leaving the second unchanged, but this is inconsistent with the case for "$\cdot$" in the regular expression derivative. What happens when the first generator's language is nullable? Luckily, our simplified form clears up the confusion: if Pair x y is in simplified form, x is not nullable. This is a simple corollary of Lemma 4.1.

Lemma 4.1. *If g is in simplified form, then either g = Pure a or $\nu\mathcal{L}[\![g]\!] = \varnothing$.*

Proof. See Appendix A. □

Remark. The derivative of a simplified generator is simplified. This follows simply from the definition, since we only use smart constructors to build the derivative generators. By induction, this also means that repeated derivatives preserve simplification.

Besides clearing up the issue with Pair, Lemma 4.1 also says that we can define *nullability* for free generators simply as:

```
ν :: FGen a → Set a
ν(Pure v) = {v}
νg        = ∅
```

A generator is nullable if and only if it can produce a result without making any more choices.

With the derivative operation defined, we can prove a concrete theorem that says our definition of derivative acts the way we expect:

Theorem 4.2 (Generator Derivative Consistency). *For all simplified free generators g and characters c,*

$$\delta_c \mathcal{L}[\![g]\!] = \mathcal{L}[\![\delta_c g]\!].$$

Proof. We again proceed by induction on the structure of g.

Case g = Void. $\emptyset = \emptyset$.

Case g = Pure a. $\emptyset = \emptyset$.

Case g = Pair x y.

$$\begin{aligned}
\delta_c \mathcal{L}[\![\text{Pair x y}]\!] &= \delta_c(\mathcal{L}[\![\text{x}]\!] \cdot \mathcal{L}[\![\text{y}]\!]) && \text{(by defn)}\\
&= \delta_c(\mathcal{L}[\![\text{x}]\!]) \cdot \mathcal{L}[\![\text{y}]\!] && \text{(by defn)}\\
&\quad + \nu\mathcal{L}[\![\text{x}]\!] \cdot \delta_c \mathcal{L}[\![\text{y}]\!] \\
&= \delta_c(\mathcal{L}[\![\text{x}]\!]) \cdot \mathcal{L}[\![\text{y}]\!] && \text{(by Lemma 4.1)}\\
&= \mathcal{L}[\![\delta_c\text{x}]\!] \cdot \mathcal{L}[\![\text{y}]\!] && \text{(by IH)}\\
&= \mathcal{L}[\![\text{Pair } (\delta_c\text{x}) \text{ y}]\!] && \text{(by defn)}\\
&= \mathcal{L}[\![\delta_c\text{Pair x y}]\!] && \text{(by defn)}
\end{aligned}$$

Case g = Map f x.

$$\begin{aligned}
\delta_c \mathcal{L}[\![\text{Map f x}]\!] &= \delta_c \mathcal{L}[\![\text{x}]\!] && \text{(by defn)}\\
&= \mathcal{L}[\![\delta_c\text{x}]\!] && \text{(by IH)}\\
&= \mathcal{L}[\![\text{Map f } (\delta_c\text{x})]\!] && \text{(by defn)}\\
&= \mathcal{L}[\![\delta_c(\text{Map f x})]\!] && \text{(by defn*)}
\end{aligned}$$

*Note that the last step follows because Map f x is assumed to be simplified, so $x \neq$ Pure a. This means that f ⟨$⟩ x is equivalent to Map f x.

Case g = Select xs. If there is no pair (c, x) in xs, then $\emptyset = \emptyset$. Otherwise,

$$\begin{aligned}
\delta_c \mathcal{L}[\![\text{Select xs}]\!] &= \delta_c\{c \cdot s \mid s \in \mathcal{L}[\![\text{x}]\!]\} && \text{(by defn)}\\
&= \mathcal{L}[\![\text{x}]\!] && \text{(by defn)}\\
&= \mathcal{L}[\![\delta_c(\text{Select xs})]\!] && \text{(by defn)}
\end{aligned}$$

Thus we have shown that the symbolic derivative of free generators is compatible with the derivative of the generator's language.[5] □

5 Generating Valid Results with Gradients

In this section, we put the theory of free generators and their derivatives into practice. We present Choice Gradient Sampling (CGS), which helps to solve the *valid generation problem* by guiding a generator to outputs that satisfy a computable precondition.

The basic intuition behind CGS is that a generator's derivative with respect to a choice c contains information about how "good" or "bad" the choice c would be—in other words, how likely that choice is to lead the generator to a valid result. In order to access this information, we can sample from $\mathcal{G}[\![\delta_c g]\!]$ a number of times and count up how many of the samples are valid. The more valid samples we get, the more likely c will lead us to a valid result at the end of generation.

5.1 The Algorithm

With this intuition in mind, we present Choice Gradient Sampling, which searches for valid results using repeated free generator *gradients* (i.e., derivatives with respect to every available choice). Given a free generator G in simplified form and a validity predicate φ, the following algorithm produces a set of outputs O such that $\forall x \in O.\ \varphi(x)$.

```
1:  g ← G
2:  V ← ∅
3:  while true do
4:      if νg ≠ ∅ then return νg ∪ V
5:      if g = Void then g ← G
6:      ∇g ← {δ_c g | c ∈ C}              ▷ ∇g is the gradient of g
7:      for δ_c g ∈ ∇g do
8:          if δ_c g = Void then
9:              V ← ∅
10:         else
11:             x_1, ..., x_N ↜ G[[δ_c g]]    ▷ Sample G[[δ_c g]]
12:             V ← {x_j | φ(x_j)}
13:         f_c ← |V|                     ▷ f_c is the fitness of c
14:         V ← V ∪ V
15:     if max_{c∈C} f_c = 0 then
16:         for c ∈ C do f_c ← 1
17:     g ↜ weightedChoice {(f_c, δ_c g) | c ∈ C}
```

(Where $N \in \mathbb{N}$ is the *sample rate constant*.)

Figure 6. Choice Gradient Sampling

[5] There is another proof of this theorem, suggested by Alexandra Silva, which uses the fact that 2^{Σ^*} is the final coalgebra, along with the observation that FGen has a $2 \times (-)^{\Sigma}$ coalgebraic structure. This approach is certainly more elegant, but it abstracts away some helpful operational intuition.

The algorithm is presented in Figure 6. The intuition from earlier plays out in lines 7–14. We take the derivative of our current generator with respect to each choice, sample values from each derivative, and then choose one of the derivatives with weights proportional to the number of valid samples from each. Since each choice is made based on the "fitness" of the associated derivative, we are likely to keep making choices that lead us to valid results.

As discussed in §2, it is important to track set $\mathcal{V}$, which keeps track of all of the valid samples that we generate while evaluating derivatives. Storing the valid samples that we find along the way ensures that no effort is wasted by the sampling process.

5.2 Modified Distributions

Before moving on, here an interesting extension to CGS based on the theory in §3.4. In that section we show that replacing a generator's distribution is as simple as pairing it with a distribution over choices (represented by the type Dist). It turns out that there is a straightforward way to adapt CGS to work for distribution-modified generators!

CGS requires that our generator structure admit three basic operations: δ_c so we can compute gradients, $\mathcal{G}[\![\cdot]\!]$ so we can sample from gradients, and ν so we know when to stop. We already showed how to define $\overline{\mathcal{G}}[\![\cdot]\!]$ for generators with modified distributions, so we only need definitions of δ_c and ν.

As a starting point, we can observe that Dist admits a simple kind of derivative:

$$\delta_c(\mathsf{h}, \mathsf{d}) = (\mathsf{h} \cdot \mathsf{c},\ \mathsf{d})$$

Intuitively, the derivative just internalizes c into the history, so future queries of the distribution take that character into account. Given that, we can further define the derivative of a pair $(\mathsf{d},\ \mathsf{g})$ of a Dist and a free generator to be:

$$\delta_c(\mathsf{d}, \mathsf{g}) = (\delta_c\mathsf{d}, \delta_c\mathsf{g})$$

Finally, to complete the construction, we can say that a modified generator's nullable set is the same as the nullable set of the underlying generator:

$$\nu(\mathsf{d}, \mathsf{g}) = \nu\mathsf{g}$$

With these definitions in hand, we can adapt our algorithm with essentially no changes!

5.3 Experiments

This section expands on the results presented in §2 and gives more details about our experimental setup and benchmarks.

5.3.1 Setup & Review. First, recall the goal of our experiments: we hope to show that free generators and their derivatives are practically useful tools by demonstrating that CGS is preferable to rejection sampling. Accordingly, we use four simple free generators in order to test four different benchmarks: **BST**, **SORTED**, **AVL**, and **STLC**. Information about each of these benchmarks is given in Table 2.

Each of these benchmarks requires a free generator as a starting point, and the exact implementation of that initial generator can have a significant impact on the final performance of generation. In order to avoid any generator cleverness complicating the final results, we chose to implement generators that followed the our inductive data types as closely as possible. For example, fgenTree, shown in §3 and used in the **BST** benchmark, follows the structure of Tree exactly. In fact, all of the generators that we use in benchmarks could be reconstructed from only type information, given appropriate meta-programming effort. For each benchmark we also chose an appropriate sample-rate constant N, based on the complexity of the particular task at hand. In general, a higher value for N means that estimates of choice fitness will be better, at the cost of increased time spent sampling. In practice this could be determined by the programmer or via heuristics based on the data type.

With a generator and a sample rate constant chosen, we ran CGS and Rejection for one minute each and recorded the unique valid values produced. Recall the totals (originally presented in Table 1):

	BST	SORTED	AVL	STLC
Rejection	9,762	6,452	156	106,282
CGS	22,286	59,436	221	298,001

Again, for the most part these numbers are quite good! The **BST**, **SORTED**, and **STLC** benchmarks all show at least a 2× increase in the number of unique valid values. (Later in this section we explore the **AVL** benchmark to understand why it does not perform as well.) In addition, we kept track of term size and constructor frequencies for all benchmarks, and we show charts like the ones in Figure 4 for all four benchmarks in Appendix C. Overall these charts show exactly the effects we would hope to see: larger terms with equivalent constructor diversity.

5.3.2 Measuring Diversity. Constructor diversity is a good starting point for understanding differences between rejection sampling and CGS, but we also sought to measure a more robust notion of value diversity—after all, in a testing scenario more diverse tests lead to higher bug-finding potential. To do this, we first note that the values that they generate are roughly isomorphic to the choice sequences that generated them. For example, in the case of **BST**, the sequence `n5l6ll` can be parsed to produce Node 5 Leaf (Node 6 Leaf Leaf) and a simple in-order traversal can recover `n5l6ll` again. This means that it is safe to measure choice sequence diversity as a proxy for value diversity.

With this in mind, we compute a *diversity metric* over our generated values by estimating the average Levenshtein

	Free Generator	Validity Condition	N	Depth
BST	Binary trees with values 0–9	Is a valid BST	50	5
SORTED	Lists with values 0–9	Is sorted	50	20
AVL	Binary trees with values and stored heights 0–9	Is a valid AVL tree (balanced)	500	5
STLC	Arbitrary ASTs for λ-terms	Is well-typed	400	5

Table 2. Overview of benchmarks.

distance [13] between pairs of choice sequences in the generated results. Computing the true mean would be computationally infeasible, so we settle for the mean of a sample of 3000 pairs from each set of valid values. The results are summarized in Table 3.

	BST	**SORTED**	**AVL**	**STLC**
Rej.	7.72(1.68)	4.77(1.14)	4.53(2.08)	12.31(4.63)
CGS	8.85(1.95)	7.34(2.02)	4.43(2.00)	13.64(4.83)

Table 3. Average Levenshtein distance between pairs of choice sequences.

These results are not as dramatic as we had hoped, with diversity only increasing by around 10% for **STLC** and around the same for **BST**. One explanation for this effect might come down to the fact that CGS retains so many of its samples. Late in the algorithm, when a large prefix of choices is already fixed, samples from the derivative generators will be quite similar. This likely results in some clusters of inputs that are all valid, but that only explore one particular shape of input.

All of that said, CGS is still promising. To start, it is already common practice to test clusters of similar inputs in certain fuzzing contexts [10], so the fact that CGS does this is not unusual. In fact, this method has been shown to be effective at finding bugs in some cases. Additionally, for most of our benchmarks (again, we return to **AVL** in a moment) CGS does increase diversity of tests; combined with the sheer number of valid inputs available, this means that CGS covers a slightly larger space of tests much more thoroughly. This effect should lead to better bug-finding in testing scenarios.

5.3.3 The Problem with AVL. Of course, the outlier in all of these results seems to be the **AVL** benchmark. CGS only manages to find a modest number of extra valid AVL trees, and their pairwise diversity is actually slightly worse than that of rejection sampling. Why might this be? We suspect that this is effect arises because AVL trees are so difficult to find randomly. Balanced binary search trees are hard to generate on their own, and AVL trees are even more difficult because the generator must guess the correct height to cache at each node. This is why rejection sampling only finds 156 AVL trees in the time it takes to find 9,762 binary search trees.

The problem with AVL trees being so hard to generate is that CGS unlikely find *any* valid trees while sampling. In particular, the check in line 15 of Figure 3 is often true, meaning that choices made uniformly at random rather than guided by the fitness of the appropriate derivatives. We could mitigate this problem by significantly increasing the sample rate constant N, but then sampling time would likely dominate generation time and result in worse performance overall.

Ultimately this failure is disappointing, but not wholly surprising—CGS approximates generator fitness via sampling, and that approximation cannot always be accurate. For now it seems that especially hard-to-satisfy predicates are out of reach for this specific algorithm. Still, gradient-based algorithms might not all fail in this way. In §7 we discuss ideas for alternative algorithms that may perform better in tricky cases.

6 Related Work

In this section we discuss some other work on the valid generation problem, comparing it to ours along various dimensions.

To start, the valid generation problem need not be solved automatically. The domain specific generator languages provided by QuickCheck [8] make it easier to write manual generators that produce valid inputs by construction. We avoid manual approaches like this in the hopes of making techniques like property-based testing more accessible to software engineers who do not have experience writing their own generators.

Languages like Luck [9] provide a sort of middle-ground solution; users are still required to put in some effort, but they are able to define generators and validity predicates at the same time. Again, this is a great solution, but we want something more automated.

When validity predicates are expressed as inductive relations, approaches like the one in *Generating Good Generators for Inductive Relations* [11] are extremely powerful. This solution is actually sufficiently automatic for our needs, but most programming languages cannot express inductive relations that capture the kinds of preconditions that software engineers care about.

Some approaches have tried to use machine learning to automatically generate valid inputs. Learn&Fuzz [6] generates valid PDF documents using a recurrent neural network. While the results are promising, this solution seems to work best when a large corpus of inputs is already available and the validity condition is more structural than semantic. In the

same vein, RLCheck [16] uses reinforcement learning to guide a generator to valid inputs. We hope to incorporate ideas from RLCheck into this work in the future, but we felt that getting the theory of free generators right was a critical first step.

In, *Generating constrained random data with uniform distribution* [3], Claessen et al. present a structure that is superficially similar to our free generator structure, but which is used in a very different way. They primarily use the syntactic structure of their generators (they call them "Spaces") to control the size distribution of the outputs; in particular, Spaces do not make choice information explicit in the way free generators do. Claessen et al.'s generation approach uses Haskell's laziness, rather than derivatives and sampling, to prune unhelpful paths in the generation process. It seems plausible that we could incorporate some of these ideas into our work to improve performance and give finer control over size distributions.

Finally, while it does not explicitly aim to solve the valid generation problem, Clotho [5] is an interesting point in the generator design space.

7 Future Directions

There are a number of exciting paths forward from this work: some continue our theoretical exploration, while others look towards algorithmic improvements that would be incredibly useful in practice.

7.1 Bidirectional Free Generators

We believe that we have only scratched the surface of what is possible with free generators. Making choices explicit opens the door for other transformations and interpretations that take advantage of the extra information. One concrete idea would be to merge the theory of free generators with the emerging theory of *ungenerators* [7]. That work expresses generators that can be run both forward (to generate values as usual) and *backward*. In the backward direction, the program takes a value that the generator might have generated and "un-generates" it to give a sequence of choices that the generator might have made when generating that value.

The free generator formalism is quite compatible with these ideas—since free generators make choices explicit, turning one into a bidirectional generator that can both generate and ungenerate should be fairly straightforward. From there, we can build on the ideas in the ungenerators work and use the backward direction of the generator to learn a distribution of choices that approximates some user-provided samples of "desirable" values. Used in conjunction with the extended algorithm from §5.2, this would give a better starting point for generation with little extra work from the user.

7.2 Algorithmic Optimizations

In §5.3.3, we uncover some problems with the Choice Gradient Sampling algorithm. Recall that because CGS evaluates derivatives via sampling, it does poorly on when validity conditions are particularly difficult to satisfy. This begs the question: might it be possible to evaluate the fitness of a derivative without naïvely sampling?

One potential angle involves staging the sampling process. Given a free generator with a depth parameter, first evaluate choices on generators of size 1, then evaluate choices with size 2, etc. These intermediate stages will make gradient sampling more successful at larger sizes, and might significantly improve the results on benchmarks like **AVL**. Unfortunately, this kind of approach might perform poorly on benchmarks like **STLC** where the validity condition is not uniform: size-1 generators would avoid generating variables, leading larger generators to avoid variables as well. In any case, we think this design space is worth exploring.

7.3 Making Choices with Neural Networks

Another algorithmic optimization is considerably farther afield: we think it may be possible to use recurrent neural networks (RNNs) to improve our generation procedure.

As Choice Gradient Sampling makes choices, it generates a lot of useful data about the frequencies with which choices should be made. Specifically, every iteration of the algorithm produces a pair of a history and a distribution over next choices that looks something like:

$$\mathsf{abcca} \mapsto \{\mathsf{a} : 0.3, \mathsf{b} : 0.7, \mathsf{c} : 0.0\}$$

In the course of CGS, this information is used once (to make the next choice) and then forgotten—what if there was a way to learn from it? Pairs like this could be used to train an RNN to make choices that are similar to the ones made by CGS.

There are still plenty of details to work out, including network architecture, hyper-parameters, etc., but given sufficient performance, we could run CGS for a while, then train the model, and after that point only use the model to generate valid data. Staging things this way would recover some of the time that is currently wasted by the constant sampling of derivative generators. One could imagine a user writing a definition of a type and a predicate for that type, and then setting the model to train while they work on their algorithm. By the time the algorithm is finished and ready to test, the RNN model would be trained and ready to produce valid test inputs. A workflow like this could significantly increase adoption of property-based testing in industry and give developers more control over the quality of their software.

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Appendix

A Proof of Lemma 4.1

Lemma 4.1. *If g is in simplified form, then either $g = \mathit{Pure}\ a$ or $\nu\mathcal{L}[\![g]\!] = \emptyset$.*

Proof. We proceed by induction on the structure of g.

Case g = Void. Trivial.
Case g = Pure a. Trivial.
Case g = Pair x y. By our inductive hypothesis, x = Pure a or $\nu\mathcal{L}[\![\mathsf{x}]\!] = \emptyset$.
Since the smart constructor $\otimes$ never constructs a Pair with Pure on the left, it must be that $\nu\mathcal{L}[\![\mathsf{x}]\!] = \emptyset$.
Therefore, it must be the case that $\nu\mathcal{L}[\![\mathsf{Pair\ x\ y}]\!] = \emptyset$.
Case g = Map f x.
Similarly to the previous case, our inductive hypothesis and simplification assumptions imply that $\nu\mathcal{L}[\![\mathsf{x}]\!] = \emptyset$.
Therefore, $\nu\mathcal{L}[\![\mathsf{Map\ f\ y}]\!] = \emptyset$.
Case g = Select xs.
It is always the case that $\nu\mathcal{L}[\![\mathsf{Select\ xs}]\!] = \emptyset$.

Thus, we have shown that every simplified free generator is either Pure a or has an empty nullable set. □

B Proof of Theorem 3.4

Lemma B.1. *Pairing two parsers and mapping over the concatenation of the associated choice distributions is equal to a function of the two parsers mapped over the distributions individually. Specifically, for all simplified free generators* x *and* y*,*

$$\begin{aligned}((\lambda x\ y \to (x,y))\ \langle\$\rangle\ \mathcal{P}[\![x]\!]\ \langle\circledast\rangle\ \mathcal{P}[\![y]\!])\ \langle\$\rangle((\cdot)\ \langle\$\rangle\ C[\![x]\!]\ \langle\circledast\rangle\ C[\![y]\!]) \equiv (\lambda a_\perp\ b_\perp \to \textbf{\textit{case}}\ (a_\perp, b_\perp)\ \textbf{\textit{of}}\\ (\mathit{Just}\ (a,\_), \mathit{Just}\ (b,\_)) \to \mathit{Just}\ ((a,b),\varepsilon)\\ \_ \to \mathit{Nothing})\\ \langle\$\rangle(\mathcal{P}[\![x]\!]\ \langle\$\rangle\ C[\![x]\!])\ \langle\circledast\rangle(\mathcal{P}[\![y]\!]\ \langle\$\rangle\ C[\![y]\!])\end{aligned}$$

Proof. First, note that for any simplified generator, g, if $C[\![g]\!]$ generates a string s, for any other string t $\mathcal{P}[\![g]\!]\ (s \cdot t) = \mathsf{Just}\ (a, t)$ for some value a. This can be shown by induction on the structure of g.
Now, assume $C[\![\mathsf{x}]\!]$ generates a string s, and $C[\![\mathsf{y}]\!]$ generates t. This means that $(\cdot)\ \langle\$\rangle\ C[\![\mathsf{x}]\!]\ \langle\circledast\rangle\ C[\![\mathsf{y}]\!]$ generates $s \cdot t$.
By the above fact, it is simple to show that both sides of the above equation simplify to $\mathsf{Just}\ ((a,b),\varepsilon)$ for some values a and b that depend on the particular interpretations of x and y.
Since this is true for any s and t that the choice distributions generate, the desired fact holds. □

Theorem 3.4. *Every simplified free generator can be factored coherently into a parser and a distribution over choice sequences. In other words, for all simplified free generators $g \neq$ Void,*

$$\mathcal{P}[\![g]\!]\ \langle\$\rangle\ C[\![g]\!] \equiv (\lambda x \to \mathit{Just}\ (x,\varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![g]\!].$$

Proof. We proceed by induction on the structure of g.

Case g = Pure a.

$$\begin{aligned}\mathcal{P}[\![\mathsf{Pure\ a}]\!]\ \langle\$\rangle\ C[\![\mathsf{Pure\ a}]\!] &\equiv \mathsf{pure}\ (\mathsf{Just}\ (\mathsf{a},\varepsilon)) && \text{(by defn)}\\ &\equiv (\lambda x \to \mathsf{Just}\ (x,\varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\mathsf{Pure\ a}]\!] && \text{(by defn)}\end{aligned}$$

Case g = Pair x y.

$$
\begin{aligned}
\mathcal{P}[\![\text{Pair x y}]\!]\ \langle\$\rangle\ \mathcal{C}[\![\text{Pair x y}]\!] &\equiv ((\lambda x\ y \to (x, y))\ \langle\$\rangle\ \mathcal{P}[\![\text{x}]\!]\ \langle*\rangle\ \mathcal{P}[\![\text{y}]\!])\ \langle\$\rangle ((\cdot)\ \langle\$\rangle\ \mathcal{C}[\![\text{x}]\!]\ \langle*\rangle\ \mathcal{C}[\![\text{y}]\!]) && \text{(by defn)}\\
&\equiv (\lambda a_\perp\ b_\perp \to \textbf{case}\ (a_\perp, b_\perp)\ \textbf{of}\\
&\qquad (\text{Just}\ (a, \_), \text{Just}\ (b, \_)) \to \text{Just}\ ((a, b), \varepsilon)\\
&\qquad \_ \to \text{Nothing})\\
&\quad \langle\$\rangle (\mathcal{P}[\![\text{x}]\!]\ \langle\$\rangle\ \mathcal{C}[\![\text{x}]\!])\ \langle*\rangle (\mathcal{P}[\![\text{y}]\!]\ \langle\$\rangle\ \mathcal{C}[\![\text{y}]\!]) && \text{(by Lemma B.1)}\\
&\equiv (\lambda a_\perp\ b_\perp \to \textbf{case}\ (a_\perp, b_\perp)\ \textbf{of}\\
&\qquad (\text{Just}\ (a, \_), \text{Just}\ (b, \_)) \to \text{Just}\ ((a, b), \varepsilon)\\
&\qquad \_ \to \text{Nothing})\\
&\quad \langle\$\rangle ((\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{x}]\!])\ \langle*\rangle ((\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{y}]\!]) && \text{(by IH)}\\
&\equiv (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle ((\lambda x\ y \to (x, y))\ \langle\$\rangle\ \mathcal{G}[\![\text{x}]\!]\ \langle*\rangle\ \mathcal{G}[\![\text{y}]\!]) && \text{(by app. properties)}\\
&\equiv (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{Pair x y}]\!] && \text{(by defn)}
\end{aligned}
$$

Case g = Map f x.

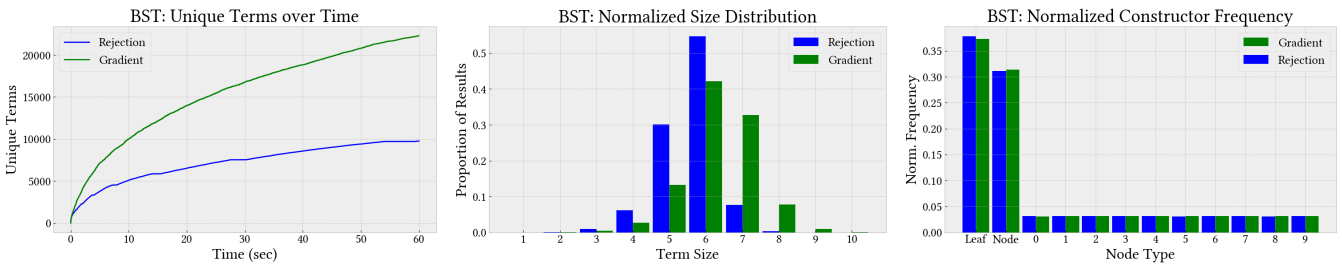
$$
\begin{aligned}
\mathcal{P}[\![\text{Map f x}]\!]\ \langle\$\rangle\ \mathcal{C}[\![\text{Map f x}]\!] &\equiv (\text{f}\ \langle\$\rangle\ \mathcal{P}[\![\text{x}]\!])\ \langle\$\rangle\ \mathcal{C}[\![x]\!] && \text{(by defn)}\\
&\equiv \text{f}\ \langle\$\rangle (\mathcal{P}[\![\text{x}]\!]\ \langle\$\rangle\ \mathcal{C}[\![x]\!]) && \text{(by functor properties)}\\
&\equiv \text{f}\ \langle\$\rangle ((\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{x}]\!]) && \text{(by IH)}\\
&\equiv (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle (\text{f}\ \langle\$\rangle\ \mathcal{G}[\![\text{x}]\!]) && \text{(by functor properties)}\\
&\equiv (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{Map f x}]\!] && \text{(by defn)}
\end{aligned}
$$

Case g = Select xs.

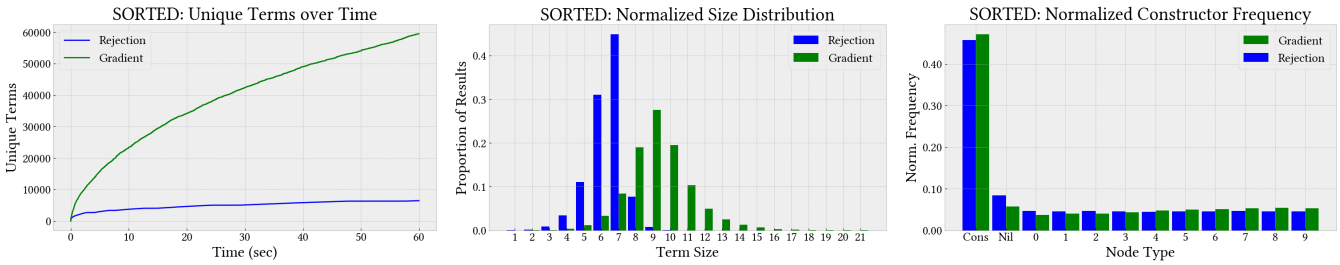
$$
\begin{aligned}
\mathcal{P}[\![\text{Select xs}]\!]\ \langle\$\rangle\ \mathcal{C}[\![\text{Select xs}]\!] &\equiv (\text{choice}\ (\text{map}\ (\lambda(c, \text{x}) \to (c, \mathcal{P}[\![\text{x}]\!]))\ \text{xs}))\\
&\qquad \langle\$\rangle\ \text{oneof}\ (\text{map}\ (\lambda(c, \text{x}) \to (c\cdot)\ \langle\$\rangle\ \mathcal{C}[\![\text{x}]\!])\ \text{xs}) && \text{(by defn)}\\
&\equiv \text{oneof}\ (\text{map}\ (\lambda(c, \text{x}) \to\\
&\qquad (\text{choice}\ (\text{map}\ (\lambda(c, \text{x}) \to (c, \mathcal{P}[\![\text{x}]\!]))\ \text{xs})) \circ (c\cdot)\ \langle\$\rangle\ \mathcal{C}[\![\text{x}]\!]\\
&\quad)\ \text{xs}) && \text{(by generator properties)}\\
&\equiv \text{oneof}\ (\text{map}\ (\lambda(\_, \text{x}) \to \mathcal{P}[\![\text{x}]\!]\ \langle\$\rangle\ \mathcal{C}[\![\text{x}]\!])\ \text{xs}) && \text{(by parser properties)}\\
&\equiv \text{oneof}\ (\text{map}\ (\lambda(\_, \text{x}) \to (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{x}]\!])\ \text{xs}) && \text{(by IH)}\\
&\equiv (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \text{oneof}\ (\text{map}\ (\lambda(\_, \text{x}) \to \mathcal{G}[\![\text{x}]\!])\ \text{xs}) && \text{(by generator properties)}\\
&\equiv (\lambda x \to \text{Just}\ (x, \varepsilon))\ \langle\$\rangle\ \mathcal{G}[\![\text{Select xs}]\!] && \text{(by defn)}
\end{aligned}
$$

Thus, generators can be coherently factored into a parser and a distribution. □

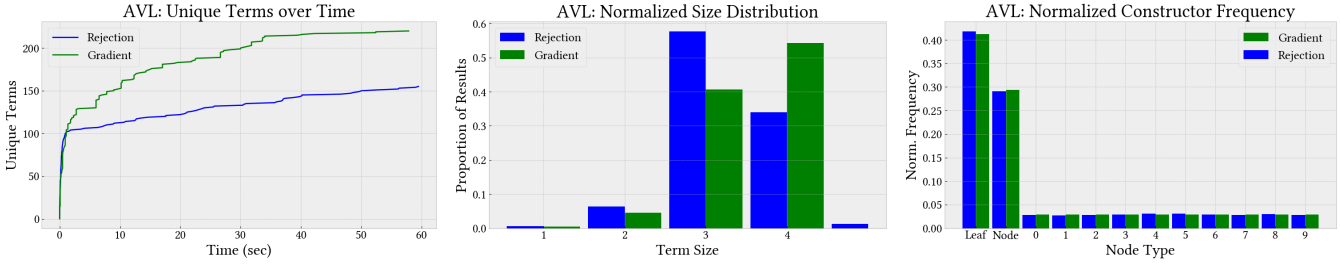
C Full Experimental Results



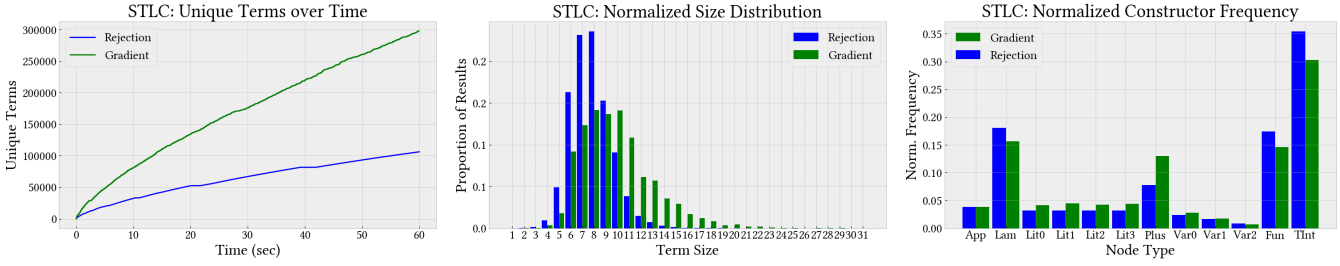
BST Charts



SORTED Charts



AVL Charts



STLC Charts