XMSS: eXtended Merkle Signature Scheme

Abstract

This note describes the eXtended Merkle Signature Scheme (XMSS), a hash-based digital signature system that is based on existing descriptions in scientific literature. This note specifies Winternitz One-Time Signature Plus (WOTS+), a one-time signature scheme; XMSS, a single-tree scheme; and XMSS^MT, a multi-tree variant of XMSS. Both XMSS and XMSS^MT use WOTS+ as a main building block. XMSS provides cryptographic digital signatures without relying on the conjectured hardness of mathematical problems. Instead, it is proven that it only relies on the properties of cryptographic hash functions. XMSS provides strong security guarantees and is even secure when the collision resistance of the underlying hash function is broken. It is suitable for compact implementations, is relatively simple to implement, and naturally resists side-channel attacks. Unlike most other signature systems, hash-based signatures can so far withstand known attacks using quantum computers.
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1. Introduction

A (cryptographic) digital signature scheme provides asymmetric message authentication. The key generation algorithm produces a key pair consisting of a private and a public key. A message is signed using a private key to produce a signature. A message/signature pair can be verified using a public key. A One-Time Signature (OTS) scheme allows using a key pair to sign exactly one message securely. A Many-Time Signature (MTS) system can be used to sign multiple messages.

OTS schemes, and MTS schemes composed from them, were proposed by Merkle in 1979 [Merkle83]. They were well-studied in the 1990s and have regained interest from the mid 2000s onwards because of their resistance against quantum-computer-aided attacks. These kinds of signature schemes are called hash-based signature schemes as they are built out of a cryptographic hash function. Hash-based signature schemes generally feature small private and public keys as well as fast signature generation and verification; however, they also feature large signatures and relatively slow key generation. In addition, they are suitable for compact implementations that benefit various applications and are naturally resistant to most kinds of side-channel attacks.

Some progress has already been made toward introducing and standardizing hash-based signatures. Buchmann, Dahmen, and Huelsing proposed the eXtended Merkle Signature Scheme (XMSS) [BDH11], which offers better efficiency than Merkle’s original scheme and a modern security proof in the standard model. McGrew, Curcio, and Fluhrer authored an Internet-Draft [MCF18] specifying the Leighton–Micali Signature (LMS) scheme, which builds on the seminal works by Lamport, Diffie, Winternitz, and Merkle, taking a different approach than XMSS and relying entirely on security arguments in the random oracle model. Very recently, the stateless hash-based signature scheme SPHINCS was introduced [BHH15], with the intent of being easier to deploy in current applications. A reasonable next step toward introducing hash-based signatures is to complete the specifications of the basic algorithms -- LMS, XMSS, SPHINCS, and/or variants.

The eXtended Merkle Signature Scheme (XMSS) [BDH11] is the latest stateful hash-based signature scheme. It has the smallest signatures out of such schemes and comes with a multi-tree variant that solves the problem of slow key generation. Moreover, it can be shown that XMSS is secure, making only mild assumptions on the underlying hash function. In particular, it is not required that the cryptographic hash function is collision-resistant for the security of XMSS. Improvements upon XMSS, as described in [HRS16], are part of this note.
This document describes a single-tree and a multi-tree variant of XMSS. It also describes WOTS+, a variant of the Winternitz OTS scheme introduced in [Huelsing13] that is used by XMSS. The schemes are described with enough specificity to ensure interoperability between implementations.

This document is structured as follows. Notation is introduced in Section 2. Section 3 describes the WOTS+ signature system. MTS schemes are defined in Section 4: the eXtended Merkle Signature Scheme (XMSS) in Section 4.1 and its multi-tree variant (XMSS^MT) in Section 4.2. Parameter sets are described in Section 5. Section 6 describes the rationale behind choices in this note. Section 7 gives information about the reference code. The IANA registry for these signature systems is described in Section 8. Finally, security considerations are presented in Section 9.

1.1. CFRG Note on Post-Quantum Cryptography

All post-quantum algorithms documented by the Crypto Forum Research Group (CFRG) are today considered ready for experimentation and further engineering development (e.g., to establish the impact of performance and sizes on IETF protocols). However, at the time of writing, we do not have significant deployment experience with such algorithms.

Many of these algorithms come with specific restrictions, e.g., change of classical interface or less cryptanalysis of proposed parameters than established schemes. CFRG has consensus that all documents describing post-quantum technologies include the above paragraph and a clear additional warning about any specific restrictions, especially as those might affect use or deployment of the specific scheme. That guidance may be changed over time via document updates.

Additionally, for XMSS:

CFRG consensus is that we are confident in the cryptographic security of the signature schemes described in this document against quantum computers, given the current state of the research community's knowledge about quantum algorithms. Indeed, we are confident that the security of a significant part of the Internet could be made dependent on the signature schemes defined in this document, if developers take care of the following.

In contrast to traditional signature schemes, the signature schemes described in this document are stateful, meaning the secret key changes over time. If a secret key state is used twice, no cryptographic security guarantees remain. In consequence, it becomes
feasible to forge a signature on a new message. This is a new property that most developers will not be familiar with and requires careful handling of secret keys. Developers should not use the schemes described here except in systems that prevent the reuse of secret key states.

Note that the fact that the schemes described in this document are stateful also implies that classical APIs for digital signatures cannot be used without modification. The API MUST be able to handle a secret key state; in particular, this means that the API MUST allow to return an updated secret key state.

1.2. Conventions Used in This Document

The key words "MUST", "MUST NOT", "REQUIRED", "SHALL", "SHALL NOT", "SHOULD", "SHOULD NOT", "RECOMMENDED", "NOT RECOMMENDED", "MAY", and "OPTIONAL" in this document are to be interpreted as described in BCP 14 [RFC2119] [RFC8174] when, and only when, they appear in all capitals, as shown here.

2. Notation

2.1. Data Types

Bytes and byte strings are the fundamental data types. A byte is a sequence of eight bits. A single byte is denoted as a pair of hexadecimal digits with a leading "0x". A byte string is an ordered sequence of zero or more bytes and is denoted as an ordered sequence of hexadecimal characters with a leading "0x". For example, 0xe534f0 is a byte string of length 3. An array of byte strings is an ordered, indexed set starting with index 0 in which all byte strings have identical length. We assume big-endian representation for any data types or structures.

2.2. Functions

If x is a non-negative real number, then we define the following functions:

- ceil(x): returns the smallest integer greater than or equal to x.
- floor(x): returns the largest integer less than or equal to x.
- lg(x): returns the logarithm to base 2 of x.
2.3. Operators

When a and b are integers, mathematical operators are defined as follows:

^ : a ^ b denotes the result of a raised to the power of b.

* : a * b denotes the product of a and b. This operator is sometimes omitted in the absence of ambiguity, as in usual mathematical notation.

/ : a / b denotes the quotient of a by non-zero b.

% : a % b denotes the non-negative remainder of the integer division of a by b.

+ : a + b denotes the sum of a and b.

- : a - b denotes the difference of a and b.

++ : a++ denotes incrementing a by 1, i.e., a = a + 1.

<< : a << b denotes a logical left shift with b being non-negative, i.e., a * 2^b.

>> : a >> b denotes a logical right shift with b being non-negative, i.e., floor(a / 2^b).

The standard order of operations is used when evaluating arithmetic expressions.

Arrays are used in the common way, where the i^{th} element of an array A is denoted A[i]. Byte strings are treated as arrays of bytes where necessary: if X is a byte string, then X[i] denotes its i^{th} byte, where X[0] is the leftmost byte.

If A and B are byte strings of equal length, then:

- A AND B denotes the bitwise logical conjunction operation.
- A XOR B denotes the bitwise logical exclusive disjunction operation.

When B is a byte and i is an integer, then B >> i denotes the logical right-shift operation.
If X is an x-byte string and Y a y-byte string, then X || Y denotes the concatenation of X and Y, with X || Y = X[0] ... X[x-1] Y[0] ... Y[y-1].

2.4. Integer-to-Byte Conversion

If x and y are non-negative integers, we define Z = toByte(x, y) to be the y-byte string containing the binary representation of x in big-endian byte order.

2.5. Hash Function Address Scheme

The schemes described in this document randomize each hash function call. This means that aside from the initial message digest, a different key and different bitmask is used for each hash function call. These values are pseudorandomly generated using a pseudorandom function that takes a key SEED and a 32-byte address ADRS as input and outputs an n-byte value, where n is the security parameter. Here we explain the structure of address ADRS and propose setter methods to manipulate the address. We explain the generation of the addresses in the following sections where they are used.

The schemes in the next two sections use two kinds of hash functions parameterized by security parameter n. For the hash tree constructions, a hash function that maps an n-byte key and 2n-byte inputs to n-byte outputs is used. To randomize this function, 3n bytes are needed -- n bytes for the key and 2n bytes for a bitmask. For the OTS scheme constructions, a hash function that maps n-byte keys and n-byte inputs to n-byte outputs is used. To randomize this function, 2n bytes are needed -- n bytes for the key and n bytes for a bitmask. Consequently, three addresses are needed for the first function and two addresses for the second one.

There are three different types of addresses for the different use cases. One type is used for the hashes in OTS schemes, one is used for hashes within the main Merkle tree construction, and one is used for hashes in the L-trees. The latter is used to compress one-time public keys. All these types share as much format as possible. In the remainder of this section, we describe these types in detail.

The structure of an address complies with word borders, with a word being 32 bits long in this context. Only the tree address is too long to fit a single word, but it can fit a double word. An address is structured as follows. It always starts with a layer address of one word in the most significant bits, followed by a tree address of two words. Both addresses are needed for the multi-tree variant (see Section 4.2) and describe the position of a tree within a multi-tree. They are therefore set to zero in single-tree applications. For
multi-tree hash-based signatures, the layer address describes the height of a tree within the multi-tree, starting from height zero for trees at the bottom layer. The tree address describes the position of a tree within a layer of a multi-tree starting with index zero for the leftmost tree. The next word defines the type of the address. It is set to 0 for an OTS address, to 1 for an L-tree address, and to 2 for a hash tree address. Whenever the type word of an address is changed, all following words should be initialized with 0 to prevent non-zero values in unused padding words.

We first describe the OTS address case. In this case, the type word is followed by an OTS address word that encodes the index of the OTS key pair within the tree. The next word encodes the chain address followed by a word that encodes the address of the hash function call within the chain. The last word, called keyAndMask, is used to generate two different addresses for one hash function call. The word is set to zero to generate the key. To generate the n-byte bitmask, the word is set to one.

<table>
<thead>
<tr>
<th>layer address (32 bits)</th>
</tr>
</thead>
<tbody>
<tr>
<td>tree address (64 bits)</td>
</tr>
<tr>
<td>-------------------------</td>
</tr>
<tr>
<td>type = 0 (32 bits)</td>
</tr>
<tr>
<td>-------------------------</td>
</tr>
<tr>
<td>OTS address (32 bits)</td>
</tr>
<tr>
<td>-------------------------</td>
</tr>
<tr>
<td>chain address (32 bits)</td>
</tr>
<tr>
<td>-------------------------</td>
</tr>
<tr>
<td>hash address (32 bits)</td>
</tr>
<tr>
<td>-------------------------</td>
</tr>
<tr>
<td>keyAndMask (32 bits)</td>
</tr>
<tr>
<td>-------------------------</td>
</tr>
</tbody>
</table>

An OTS Hash Address

We now discuss the L-tree case, which means that the type word is set to one. In that case, the type word is followed by an L-tree address word that encodes the index of the leaf computed with this L-tree. The next word encodes the height of the node being input for the next computation inside the L-tree. The following word encodes the index of the node at that height, inside the L-tree. This time, the last word, keyAndMask, is used to generate three different addresses for one function call. The word is set to zero to generate the key. To generate the most significant n bytes of the 2n-byte bitmask, the word is set to one. The least significant bytes are generated using the address with the word set to two.
An L-tree Address

We now describe the remaining type for the main tree hash addresses. In this case, the type word is set to two, followed by a zero padding of one word. The next word encodes the height of the tree node being input for the next computation, followed by a word that encodes the index of this node at that height. As for the L-tree addresses, the last word, keyAndMask, is used to generate three different addresses for one function call. The word is set to zero to generate the key. To generate the most significant n bytes of the 2n-byte bitmask, the word is set to one. The least significant bytes are generated using the address with the word set to two.

A Hash Tree Address
All fields within these addresses encode unsigned integers. When describing the generation of addresses we use setter methods that take positive integers and set the bits of a field to the binary representation of that integer of the length of the field. We furthermore assume that the setType() method sets the four words following the type word to zero.

2.6. Strings of Base w Numbers

A byte string can be considered as a string of base w numbers, i.e., integers in the set \( \{0, \ldots, w - 1\} \). The correspondence is defined by the function \( \text{base}_w(X, w, \text{out}_\text{len}) \) (Algorithm 1) as follows. If \( X \) is a len_X-byte string, and \( w \) is a member of the set \( \{4, 16\} \), then \( \text{base}_w(X, w, \text{out}_\text{len}) \) outputs an array of \( \text{out}_\text{len} \) integers between 0 and \( w - 1 \). The length \( \text{out}_\text{len} \) is REQUIRED to be less than or equal to \( 8 \times \text{len}_X / \log(w) \).

**Algorithm 1: base_w**

Input: len_X-byte string X, int w, output length out_len
Output: out_len int array basew

```c
int in = 0;
int out = 0;
unsigned int total = 0;
int bits = 0;
int consumed;

for ( consumed = 0; consumed < out_len; consumed++ ) {
    if ( bits == 0 ) {
        total = X[in];
        in++;
        bits += 8;
    } else {
        bits -= \log(w);
        basew[out] = (total >> bits) AND (w - 1);
        out++;
    }
}
return basew;
```

For example, if \( X \) is the (big-endian) byte string 0x1234, then \( \text{base}_w(X, 16, 4) \) returns the array \( a = \{1, 2, 3, 4\} \).
2.7. Member Functions

To simplify algorithm descriptions, we assume the existence of member functions. If a complex data structure like a public key PK contains a value X, then `getX(PK)` returns the value of X for this public key. Accordingly, `setX(PK, X, Y)` sets value X in PK to the value held by Y. Since camelCase is used for member function names, a value z may be referred to as Z in the function name, e.g., `getZ`.
3. Primitives

3.1. WOTS+: One-Time Signatures

This section describes the WOTS+ system in a manner similar to that in [Huelsing13]. WOTS+ is an OTS scheme; while a private key can be used to sign any message, each private key MUST be used only once to sign a single message. In particular, if a private key is used to sign two different messages, the scheme becomes insecure.

This section starts with an explanation of parameters. Afterwards, the so-called chaining function, which forms the main building block of the WOTS+ scheme, is explained. A description of the algorithms for key generation, signing, and verification follows. Finally, pseudorandom key generation is discussed.

3.1.1. WOTS+ Parameters

WOTS+ uses the parameters n and w; they both take positive integer values. These parameters are summarized as follows:

n: the message length as well as the length of a private key, public key, or signature element in bytes.

w: the Winternitz parameter; it is a member of the set {4, 16}.

The parameters are used to compute values \( \text{len} \), \( \text{len}_1 \), and \( \text{len}_2 \):

\[
\text{len} = \text{len}_1 + \text{len}_2,
\]

with \( \text{len}_1 = \text{ceil}(8n / \lg(w)) \) and \( \text{len}_2 = \text{floor}(\lg(\text{len}_1 \times (w - 1)) / \lg(w)) + 1 \).

The value of n is determined by the cryptographic hash function used for WOTS+. The hash function is chosen to ensure an appropriate level of security. The value of n is the input length that can be processed by the signing algorithm. It is often the length of a message digest. The parameter w can be chosen from the set \{4, 16\}. A larger value of w results in shorter signatures but slower overall signing operations; it has little effect on security. Choices of w are limited to the values 4 and 16 since these values yield optimal trade-offs and easy implementation.

WOTS+ parameters are implicitly included in algorithm inputs as needed.
3.1.1.1. WOTS+ Functions

The WOTS+ algorithm uses a keyed cryptographic hash function F. F accepts and returns byte strings of length n using keys of length n. More detail on specific instantiations can be found in Section 5. Security requirements on F are discussed in Section 9. In addition, WOTS+ uses a pseudorandom function PRF. PRF takes as input an n-byte key and a 32-byte index and generates pseudorandom outputs of length n. More detail on specific instantiations can be found in Section 5. Security requirements on PRF are discussed in Section 9.

3.1.2. WOTS+ Chaining Function

The chaining function (Algorithm 2) computes an iteration of F on an n-byte input using outputs of PRF. It takes an OTS hash address as input. This address will have the first six 32-bit words set to encode the address of this chain. In each iteration, PRF is used to generate a key for F and a bitmask that is XORed to the intermediate result before it is processed by F. In the following, ADRS is a 32-byte OTS hash address as specified in Section 2.5 and SEED is an n-byte string. To generate the keys and bitmasks, PRF is called with SEED as key and ADRS as input. The chaining function takes as input an n-byte string X, a start index i, a number of steps s, as well as ADRS and SEED. The chaining function returns as output the value obtained by iterating F for s times on input X, using the outputs of PRF.
Algorithm 2: chain - Chaining Function

Input: Input string $X$, start index $i$, number of steps $s$, seed $SEED$, address $ADRS$
Output: value of $F$ iterated $s$ times on $X$

if ($s == 0$) {
    return $X$;
} else if ($i + s > (w - 1)$) {
    return NULL;
} else {
    byte[$n$] tmp = chain($X$, $i$, $s - 1$, $SEED$, $ADRS$);

    $ADRS$.setHashAddress($i + s - 1$);
    $ADRS$.setKeyAndMask(0);
    $KEY = PRF(SEED, ADRS);$
    $ADRS$.setKeyAndMask(1);
    $BM = PRF(SEED, ADRS);$

    tmp = $F(KEY, tmp XOR BM)$;
    return tmp;
}

3.1.3. WOTS+ Private Key

The private key in WOTS+, denoted by $sk$ (s for secret), is a length $len$ array of $n$-byte strings. This private key MUST be only used to sign at most one message. Each $n$-byte string MUST either be selected randomly from the uniform distribution or be selected using a cryptographically secure pseudorandom procedure. In the latter case, the security of the used procedure MUST at least match that of the WOTS+ parameters used. For a further discussion on pseudorandom key generation, see Section 3.1.7. The following pseudocode (Algorithm 3) describes an algorithm for generating $sk$.

Algorithm 3: WOTS_genSK - Generating a WOTS+ Private Key

Input: No input
Output: WOTS+ private key $sk$

for ($i = 0$; $i < len$; $i++$) {
    initialize $sk[i]$ with a uniformly random $n$-byte string;
} return $sk$;
3.1.4. WOTS+ Public Key

A WOTS+ key pair defines a virtual structure that consists of len hash chains of length w. The len n-byte strings in the private key each define the start node for one hash chain. The public key consists of the end nodes of these hash chains. Therefore, like the private key, the public key is also a length len array of n-byte strings. To compute the hash chain, the chaining function (Algorithm 2) is used. An OTS hash address ADRS and a seed SEED have to be provided by the calling algorithm. This address will encode the address of the WOTS+ key pair within a greater structure. Hence, a WOTS+ algorithm MUST NOT manipulate any parts of ADRS except for the last three 32-bit words. Please note that the SEED used here is public information also available to a verifier. The following pseudocode (Algorithm 4) describes an algorithm for generating the public key pk, where sk is the private key.

Algorithm 4: WOTS_genPK - Generating a WOTS+ Public Key From a Private Key

Input: WOTS+ private key sk, address ADRS, seed SEED
Output: WOTS+ public key pk

for ( i = 0; i < len; i++ ) {
    ADRS.setChainAddress(i);
    pk[i] = chain(sk[i], 0, w - 1, SEED, ADRS);
}
return pk;

3.1.5. WOTS+ Signature Generation

A WOTS+ signature is a length len array of n-byte strings. The WOTS+ signature is generated by mapping a message to len integers between 0 and w - 1. To this end, the message is transformed into len_1 base w numbers using the base_w function defined in Section 2.6. Next, a checksum is computed and appended to the transformed message as len_2 base w numbers using the base_w function. Note that the checksum may reach a maximum integer value of len_1 * (w - 1) * 2^8 and therefore depends on the parameters n and w. For the parameter sets given in Section 5, a 32-bit unsigned integer is sufficient to hold the checksum. If other parameter settings are used, the size of the variable holding the integer value of the checksum MUST be sufficiently large. Each of the base w integers is used to select a node from a different hash chain. The signature is formed by concatenating the selected nodes. An OTS hash address ADRS and a seed SEED have to be provided by the calling algorithm. This address will encode the address of the WOTS+ key pair within a greater structure. Hence, a WOTS+ algorithm MUST NOT manipulate any parts of
ADRS except for the last three 32-bit words. Please note that the SEED used here is public information also available to a verifier. The pseudocode for signature generation is shown below (Algorithm 5), where M is the message and sig is the resulting signature.

Algorithm 5: WOTS_sign - Generating a signature from a private key and a message

Input: Message M, WOTS+ private key sk, address ADRS, seed SEED
Output: WOTS+ signature sig

csum = 0;

// Convert message to base w
msg = base_w(M, w, len_1);

// Compute checksum
for ( i = 0; i < len_1; i++ ) {
    csum = csum + w - 1 - msg[i];
}

// Convert csum to base w
        csum = csum << ( 8 - ( ( len_2 * lg(w) ) % 8 ));
        len_2_bytes = ceil( ( len_2 * lg(w) ) / 8 );
        msg = msg || base_w(toByte(csum, len_2_bytes), w, len_2);
for ( i = 0; i < len; i++ ) {
    ADRS.setChainAddress(i);
    sig[i] = chain(sk[i], 0, msg[i], SEED, ADRS);
}
return sig;

The data format for a signature is given below.

```
+---------------------------------+
|                                 |
|           sig_ots[0]            |    n bytes
|                                 |
|                                 |
|                                 |
|                                 |
|                                 |
+---------------------------------+
|                                 |
|                                 |
|                                 |
+---------------------------------+
|                                 |
|           sig_ots[len - 1]      |    n bytes
|                                 |
+---------------------------------+

WOTS+ Signature

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3.1.6. WOTS+ Signature Verification

In order to verify a signature sig on a message M, the verifier computes a WOTS+ public key value from the signature. This can be done by "completing" the chain computations starting from the signature values, using the base w values of the message hash and its checksum. This step, called WOTS_pkFromSig, is described below in Algorithm 6. The result of WOTS_pkFromSig is then compared to the given public key. If the values are equal, the signature is accepted. Otherwise, the signature MUST be rejected. An OTS hash address ADRS and a seed SEED have to be provided by the calling algorithm. This address will encode the address of the WOTS+ key pair within a greater structure. Hence, a WOTS+ algorithm MUST NOT manipulate any parts of ADRS except for the last three 32-bit words. Please note that the SEED used here is public information also available to a verifier.

Algorithm 6: WOTS_pkFromSig - Computing a WOTS+ public key from a message and its signature

Input: Message M, WOTS+ signature sig, address ADRS, seed SEED
Output: 'Temporary' WOTS+ public key tmp_pk

csum = 0;

// Convert message to base w
msg = base_w(M, w, len_1);

// Compute checksum
for ( i = 0; i < len_1; i++ ) {
    csum = csum + w - 1 - msg[i];
}

// Convert csum to base w
len_2_bytes = ceil( ( len_2 * lg(w) ) / 8 );
msg = msg || base_w(toByte(csum, len_2_bytes), w, len_2);
for ( i = 0; i < len; i++ ) {
    ADRS.setChainAddress(i);
    tmp_pk[i] = chain(sig[i], msg[i], w - 1 - msg[i], SEED, ADRS);
}
return tmp_pk;

Note: XMSS uses WOTS_pkFromSig to compute a public key value and delays the comparison to a later point.
3.1.7. Pseudorandom Key Generation

An implementation MAY use a cryptographically secure pseudorandom method to generate the private key from a single n-byte value. For example, the method suggested in [BDH11] and explained below MAY be used. Other methods MAY be used. The choice of a pseudorandom method does not affect interoperability, but the cryptographic strength MUST match that of the used WOTS+ parameters.

The advantage of generating the private key elements from a random n-byte string is that only this n-byte string needs to be stored instead of the full private key. The key can be regenerated when needed. The suggested method from [BDH11] can be described using PRF. During key generation, a uniformly random n-byte string S is sampled from a secure source of randomness. This string S is stored as private key. The private key elements are computed as sk[i] = PRF(S, toByte(i, 32)) whenever needed. Please note that this seed S MUST be different from the seed SEED used to randomize the hash function calls. Also, this seed S MUST be kept secret. The seed S MUST NOT be a low entropy, human-memorable value since private key elements are derived from S deterministically and their confidentiality is security-critical.

4. Schemes

In this section, the eXtended Merkle Signature Scheme (XMSS) is described using WOTS+. XMSS comes in two flavors: a single-tree variant (XMSS) and a multi-tree variant (XMSS^MT). Both allow combining a large number of WOTS+ key pairs under a single small public key. The main ingredient added is a binary hash tree construction. XMSS uses a single hash tree while XMSS^MT uses a tree of XMSS key pairs.

4.1. XMSS: eXtended Merkle Signature Scheme

XMSS is a method for signing a potentially large but fixed number of messages. It is based on the Merkle signature scheme. XMSS uses four cryptographic components: WOTS+ as OTS method, two additional cryptographic hash functions H and H_msg, and a pseudorandom function PRF. One of the main advantages of XMSS with WOTS+ is that it does not rely on the collision resistance of the used hash functions but on weaker properties. Each XMSS public/private key pair is associated with a perfect binary tree, every node of which contains an n-byte value. Each tree leaf contains a special tree hash of a WOTS+ public key value. Each non-leaf tree node is computed by first concatenating the values of its child nodes, computing the XOR with a bitmask, and applying the keyed hash function H to the result. The bitmasks and the keys for the hash function H are generated from a
(public) seed that is part of the public key using the pseudorandom function PRF. The value corresponding to the root of the XMSS tree forms the XMSS public key together with the seed.

To generate a key pair that can be used to sign $2^h$ messages, a tree of height $h$ is used. XMSS is a stateful signature scheme, meaning that the private key changes with every signature generation. To prevent one-time private keys from being used twice, the WOTS+ key pairs are numbered from 0 to $(2^h) - 1$ according to the related leaf, starting from index 0 for the leftmost leaf. The private key contains an index that is updated with every signature generation, such that it contains the index of the next unused WOTS+ key pair.

A signature consists of the index of the used WOTS+ key pair, the WOTS+ signature on the message, and the so-called authentication path. The latter is a vector of tree nodes that allow a verifier to compute a value for the root of the tree starting from a WOTS+ signature. A verifier computes the root value and compares it to the respective value in the XMSS public key. If they match, the signature is declared valid. The XMSS private key consists of all WOTS+ private keys and the current index. To reduce storage, a pseudorandom key generation procedure, as described in [BDH11], MAY be used. The security of the used method MUST at least match the security of the XMSS instance.

4.1.1. XMSS Parameters

XMSS has the following parameters:

- $h$: the height (number of levels - 1) of the tree
- $n$: the length in bytes of the message digest as well as each node
- $w$: the Winternitz parameter as defined for WOTS+ in Section 3.1

There are $2^h$ leaves in the tree.

For XMSS and XMSS^MT, private and public keys are denoted by SK (S for secret) and PK, respectively. For WOTS+, private and public keys are denoted by sk (s for secret) and pk, respectively. XMSS and XMSS^MT signatures are denoted by Sig. WOTS+ signatures are denoted by sig.

XMSS and XMSS^MT parameters are implicitly included in algorithm inputs as needed.
4.1.2. XMSS Hash Functions

Besides the cryptographic hash function F and the pseudorandom function PRF required by WOTS+, XMSS uses two more functions:

- A cryptographic hash function H. H accepts n-byte keys and byte strings of length 2n and returns an n-byte string.
- A cryptographic hash function H_msg. H_msg accepts 3n-byte keys and byte strings of arbitrary length and returns an n-byte string.

More detail on specific instantiations can be found in Section 5. Security requirements on H and H_msg are discussed in Section 9.

4.1.3. XMSS Private Key

An XMSS private key SK contains 2^h WOTS+ private keys, the leaf index idx of the next WOTS+ private key that has not yet been used, SK_PRF (an n-byte key to generate pseudorandom values for randomized message hashing), the n-byte value root (which is the root node of the tree and SEED), and the n-byte public seed used to pseudorandomly generate bitmasks and hash function keys. Although root and SEED formally would be considered only part of the public key, they are needed (e.g., for signature generation) and hence are also required for functions that do not take the public key as input.

The leaf index idx is initialized to zero when the XMSS private key is created. The key SK_PRF MUST be sampled from a secure source of randomness that follows the uniform distribution. The WOTS+ private keys MUST be generated as described in Section 3.1, or, to reduce the private key size, a cryptographic pseudorandom method MUST be used as discussed in Section 4.1.11. SEED is generated as a uniformly random n-byte string. Although SEED is public, it is critical for security that it is generated using a good entropy source. The root node is generated as described below in the section on key generation (Section 4.1.7). That section also contains an example algorithm for combined private and public key generation.

For the following algorithm descriptions, the existence of a method getWOTS_SK(SK, i) is assumed. This method takes as input an XMSS private key SK and an integer i and outputs the i^th WOTS+ private key of SK.
4.1.4. Randomized Tree Hashing

To improve readability, we introduce a function RAND_HASH(LEFT, RIGHT, SEED, ADRS) (Algorithm 7) that does the randomized hashing in the tree. It takes as input two n-byte values LEFT and RIGHT that represent the left and the right halves of the hash function input, the seed SEED used as key for PRF, and the address ADRS of this hash function call. RAND_HASH first uses PRF with SEED and ADRS to generate a key KEY and n-byte bitmasks BM_0, BM_1. Then, it returns the randomized hash H(KEY, (LEFT XOR BM_0) || (RIGHT XOR BM_1)).

Algorithm 7: RAND_HASH

Input: n-byte value LEFT, n-byte value RIGHT, seed SEED, address ADRS
Output: n-byte randomized hash

ADRS.setKeyAndMask(0);
KEY = PRF(SEED, ADRS);
ADRS.setKeyAndMask(1);
BM_0 = PRF(SEED, ADRS);
ADRS.setKeyAndMask(2);
BM_1 = PRF(SEED, ADRS);

return H(KEY, (LEFT XOR BM_0) || (RIGHT XOR BM_1));

4.1.5. L-Trees

To compute the leaves of the binary hash tree, a so-called L-tree is used. An L-tree is an unbalanced binary hash tree, distinct but similar to the main XMSS binary hash tree. The algorithm ltree (Algorithm 8) takes as input a WOTS+ public key pk and compresses it to a single n-byte value pk[0]. It also takes as input an L-tree address ADRS that encodes the address of the L-tree and the seed SEED.
Algorithm 8: ltree

Input: WOTS+ public key pk, address ADRS, seed SEED
Output: n-byte compressed public key value pk[0]

unsigned int len' = len;
ADRS.setTreeHeight(0);
while ( len' > 1 ) {
    for ( i = 0; i < floor(len' / 2); i++ ) {
        ADRS.setTreeIndex(i);
        pk[i] = RAND_HASH(pk[2i], pk[2i + 1], SEED, ADRS);
    }
    if ( len' % 2 == 1 ) {
        pk[floor(len' / 2)] = pk[len' - 1];
    }
    len' = ceil(len' / 2);
    ADRS.setTreeHeight(ADRS.getTreeHeight() + 1);
}
return pk[0];

4.1.6. TreeHash

For the computation of the internal n-byte nodes of a Merkle tree, the subroutine treeHash (Algorithm 9) accepts an XMSS private key SK (including seed SEED), an unsigned integer s (the start index), an unsigned integer t (the target node height), and an address ADRS that encodes the address of the containing tree. For the height of a node within a tree, counting starts with the leaves at height zero. The treeHash algorithm returns the root node of a tree of height t with the leftmost leaf being the hash of the WOTS+ pk with index s. It is REQUIRED that s % 2^t = 0, i.e., that the leaf at index s is a leftmost leaf of a sub-tree of height t. Otherwise, the hash-addressing scheme fails. The treeHash algorithm described here uses a stack holding up to (t - 1) nodes, with the usual stack functions push() and pop(). We furthermore assume that the height of a node (an unsigned integer) is stored alongside a node’s value (an n-byte string) on the stack.
Algorithm 9: treeHash

Input: XMSS private key SK, start index s, target node height t, address ADRS
Output: n-byte root node - top node on Stack

if( s % (1 << t) != 0 ) return -1;
for ( i = 0; i < 2^t; i++ ) {
    SEED = getSEED(SK);
    ADRS.setType(0);   // Type = OTS hash address
    ADRS.setOTSAddress(s + i);
    pk = WOTS_genPK (getWOTS_SK(SK, s + i), SEED, ADRS);
    ADRS.setType(1);   // Type = L-tree address
    ADRS.setLTreeAddress(s + i);
    node = ltree(pk, SEED, ADRS);
    ADRS.setType(2);   // Type = hash tree address
    ADRS.setTreeHeight(0);
    ADRS.setTreeIndex(i + s);
    while ( Top node on Stack has same height t’ as node ) {
        ADRS.setTreeIndex((ADRS.getTreeIndex() - 1) / 2);
        node = RAND_HASH(Stack.pop(), node, SEED, ADRS);
        ADRS.setTreeHeight(ADRS.getTreeHeight() + 1);
    }
    Stack.push(node);
}
return Stack.pop();

4.1.7. XMSS Key Generation

The XMSS key pair is computed as described in XMSS_keyGen (Algorithm 10). The XMSS public key PK consists of the root of the binary hash tree and the seed SEED, both also stored in SK. The root is computed using treeHash. For XMSS, there is only a single main tree. Hence, the used address is set to the all-zero string in the beginning. Note that we do not define any specific format or handling for the XMSS private key SK by introducing this algorithm. It relates to requirements described earlier and simply shows a basic but very inefficient example to initialize a private key.
Algorithm 10: XMSS_keyGen - Generate an XMSS key pair

Input: No input
Output: XMSS private key SK, XMSS public key PK

// Example initialization for SK-specific contents
idx = 0;
for ( i = 0; i < 2^h; i++ ) {
    wots_sk[i] = WOTS_genSK();
}
initialize SK_PRF with a uniformly random n-byte string;
setSK_PRF(SK, SK_PRF);

// Initialization for common contents
initialize SEED with a uniformly random n-byte string;
setSEED(SK, SEED);
setWOTS_SK(SK, wots_sk);
ADRS = toByte(0, 32);
root = treeHash(SK, 0, h, ADRS);

SK = idx || wots_sk || SK_PRF || root || SEED;
PK = OID || root || SEED;
return (SK || PK);

The above is just an example algorithm. It is strongly RECOMMENDED to use pseudorandom key generation to reduce the private key size. Public and private key generation MAY be interleaved to save space. Particularly, when a pseudorandom method is used to generate the private key, generation MAY be done when the respective WOTS+ key pair is needed by treeHash.

The format of an XMSS public key is given below.

+---------------------------------+
|          algorithm OID           |
|                                 |
|            root node             |     n bytes
|                                 |
|              SEED                |     n bytes
+---------------------------------+
XMSS Public Key

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4.1.8. XMSS Signature

An XMSS signature is a \((4 + n + (\text{len} + h) \times n)\)-byte string consisting of:

- the index \(\text{idx\_sig}\) of the used WOTS+ key pair (4 bytes),
- a byte string \(r\) used for randomized message hashing (\(n\) bytes),
- a WOTS+ signature \(\text{sig\_ots}\) (\(\text{len} \times n\) bytes), and
- the so-called authentication path ‘auth’ for the leaf associated with the used WOTS+ key pair (\(h \times n\) bytes).

The authentication path is an array of \(h\) \(n\)-byte strings. It contains the siblings of the nodes on the path from the used leaf to the root. It does not contain the nodes on the path itself. A verifier needs these nodes to compute a root node for the tree from the WOTS+ public key. A node \(\text{Node}(x, y)\) is addressed by its position in the tree. \(\text{Node}(x, y)\) denotes the \(y\)\(^{th}\) node on level \(x\) with \(y = 0\) being the leftmost node on a level. The leaves are on level 0; the root is on level \(h\). An authentication path contains exactly one node on every layer \(0 \leq x \leq (h - 1)\). For the \(i\)\(^{th}\) WOTS+ key pair, counting from zero, the \(j\)\(^{th}\) authentication path node is:

\[ \text{Node}(j, \text{floor}(i / (2^j)) \ XOR \ 1) \]

The computation of the authentication path is discussed in Section 4.1.9.
The data format for a signature is given below.

```
+---------------------------------+    4 bytes
|                                 |
|                                 |
+---------------------------------+

index idx_sig

+---------------------------------+    n bytes
|                                 |
|                                 |
+---------------------------------+

randomness r

+---------------------------------+    len * n bytes
|                                 |
|                                 |
+---------------------------------+

WOTS+ signature sig_ots

+---------------------------------+    n bytes
|                                 |
|                                 |
+---------------------------------+

auth[0]

|   ....   |
|          |
|          |
+---------------------------------+

auth[h - 1]

XMSS Signature

4.1.9. XMSS Signature Generation

To compute the XMSS signature of a message $M$ with an XMSS private key, the signer first computes a randomized message digest using a random value $r$, $\text{idx}_\text{sig}$, the index of the WOTS+ key pair to be used, and the root value from the public key as key. Then, a WOTS+ signature of the message digest is computed using the next unused WOTS+ private key. Next, the authentication path is computed. Finally, the private key is updated, i.e., $\text{idx}$ is incremented. An implementation MUST NOT output the signature before the private key is updated.

The node values of the authentication path MAY be computed in any way. This computation is assumed to be performed by the subroutine buildAuth for the function XMSS_sign (Algorithm 12). The fastest alternative is to store all tree nodes and set the array in the signature by copying the respective nodes. The least storage-intensive alternative is to recompute all nodes for each signature.
online using the treeHash algorithm (Algorithm 9). Several
algorithms exist in between, with different time/storage trade-offs.
For an overview, see [BDS09]. A further approach can be found in
[KMN14]. Note that the details of this procedure are not relevant to
interoperability; it is not necessary to know any of these details in
order to perform the signature verification operation. The following
version of buildAuth is given for completeness. It is a simple
example for understanding, but extremely inefficient. The use of one
of the alternative algorithms is strongly RECOMMENDED.

Given an XMSS private key SK, all nodes in a tree are determined.
Their values are defined in terms of treeHash (Algorithm 9). Hence,
one can compute the authentication path as follows:

(Example) buildAuth - Compute the authentication path for the i^th
WOTS+ key pair

Input: XMSS private key SK, WOTS+ key pair index i, ADRS
Output: Authentication path auth

for (j = 0; j < h; j++) {
    k = floor(i / (2^j)) XOR 1;
    auth[j] = treeHash(SK, k * 2^j, j, ADRS);
}

We split the description of the signature generation into two main
algorithms. The first one, treeSig (Algorithm 11), generates the
main part of an XMSS signature and is also used by the multi-tree
variant XMSS^MT. XMSS_sign (Algorithm 12) calls treeSig but handles
message compression before and the private key update afterwards.

The algorithm treeSig (Algorithm 11) described below calculates the
WOTS+ signature on an n-byte message and the corresponding
authentication path. treeSig takes as input an n-byte message M’, an
XMSS private key SK, a signature index idx_sig, and an address ADRS.
It returns the concatenation of the WOTS+ signature sig_ots and
authentication path auth.
Algorithm 11: treeSig - Generate a WOTS+ signature on a message with corresponding authentication path

Input: n-byte message M', XMSS private key SK, signature index idx_sig, ADRS
Output: Concatenation of WOTS+ signature sig_ots and authentication path auth

auth = buildAuth(SK, idx_sig, ADRS);
ADRS.setType(0);  // Type = OTS hash address
ADRS.setOTSAddress(idx_sig);
sig_ots = WOTS_sign(getWOTS_SK(SK, idx_sig), M', getSEED(SK), ADRS);
Sig = sig_ots || auth;
return Sig;

The algorithm XMSS_sign (Algorithm 12) described below calculates an updated private key SK and a signature on a message M. XMSS_sign takes as input a message M of arbitrary length and an XMSS private key SK. It returns the byte string containing the concatenation of the updated private key SK and the signature Sig.

Algorithm 12: XMSS_sign - Generate an XMSS signature and update the XMSS private key

Input: Message M, XMSS private key SK
Output: Updated SK, XMSS signature Sig

idx_sig = getIdx(SK);
setIdx(SK, idx_sig + 1);
ADRS = toByte(0, 32);
byte[n] r = PRF(getSK_PRF(SK), toByte(idx_sig, 32));
byte[n] M' = H_msg(r || getRoot(SK) || (toByte(idx_sig, n)), M);
Sig = idx_sig || r || treeSig(M', SK, idx_sig, ADRS);
return (SK || Sig);

4.1.10. XMSS Signature Verification

An XMSS signature is verified by first computing the message digest using randomness r, index idx_sig, the root from PK and message M. Then the used WOTS+ public key pk_ots is computed from the WOTS+ signature using WOTS_pkFromSig. The WOTS+ public key in turn is used to compute the corresponding leaf using an L-tree. The leaf, together with index idx_sig and authentication path auth is used to compute an alternative root value for the tree. The verification succeeds if and only if the computed root value matches the one in the XMSS public key. In any other case, it MUST return fail.
As for signature generation, we split verification into two parts to allow for reuse in the XMSS^MT description. The steps also needed for XMSS^MT are done by the function XMSS_rootFromSig (Algorithm 13). XMSS_verify (Algorithm 14) calls XMSS_rootFromSig as a subroutine and handles the XMSS-specific steps.

The main part of XMSS signature verification is done by the function XMSS_rootFromSig (Algorithm 13) described below. XMSS_rootFromSig takes as input an index idx_sig, a WOTS+ signature sig_ots, an authentication path auth, an n-byte message M', seed SEED, and address ADRS. XMSS_rootFromSig returns an n-byte string holding the value of the root of a tree defined by the input data.

Algorithm 13: XMSS_rootFromSig - Compute a root node from a tree signature

```
Input: index idx_sig, WOTS+ signature sig_ots, authentication path auth, n-byte message M', seed SEED, address ADRS
Output: n-byte root value node[0]

ADRS.setType(0);   // Type = OTS hash address
ADRS.setOTSPassword(idx_sig);
pk_ots = WOTS_pkFromSig(sig_ots, M', SEED, ADRS);
ADRS.setType(1);   // Type = L-tree address
ADRS.setLTreeAddress(idx_sig);
byte[n][2] node;
node[0] = ltree(pk_ots, SEED, ADRS);
ADRS.setType(2);   // Type = hash tree address
ADRS.setTreeIndex(idx_sig);
for ( k = 0; k < h; k++ ) {
    ADRS.setTreeHeight(k);
    if ( (floor(idx_sig / (2^k)) % 2) == 0 ) {
        ADRS.setTreeIndex(ADRS.getTreeIndex() / 2);
        node[1] = RAND_HASH(node[0], auth[k], SEED, ADRS);
    } else {
        ADRS.setTreeIndex((ADRS.getTreeIndex() - 1) / 2);
        node[1] = RAND_HASH(auth[k], node[0], SEED, ADRS);
    }
    node[0] = node[1];
}
return node[0];
```

The full XMSS signature verification is depicted below (Algorithm 14). It handles message compression, delegates the root computation to XMSS_rootFromSig, and compares the result to the value in the public key. XMSS_verify takes as input an XMSS signature Sig, a
message M, and an XMSS public key PK. XMSS_verify returns true if and only if Sig is a valid signature on M under public key PK. Otherwise, it returns false.

Algorithm 14: XMSS_verify - Verify an XMSS signature using the corresponding XMSS public key and a message

Input: XMSS signature Sig, message M, XMSS public key PK
Output: Boolean

ADRS = toByte(0, 32);
byte[n] M' = H_msg(r || getRoot(PK) || (toByte(idx_sig, n)), M);

byte[n] node = XMSS_rootFromSig(idx_sig, sig_ots, auth, M', getSEED(PK), ADRS);
if ( node == getRoot(PK) ) {
    return true;
} else {
    return false;
}

4.1.11. Pseudorandom Key Generation

An implementation MAY use a cryptographically secure pseudorandom method to generate the XMSS private key from a single n-byte value. For example, the method suggested in [BDH11] and explained below MAY be used. Other methods, such as the one in [HRS16], MAY be used. The choice of a pseudorandom method does not affect interoperability, but the cryptographic strength MUST match that of the used XMSS parameters.

For XMSS, a method similar to that for WOTS+ can be used. The suggested method from [BDH11] can be described using PRF. During key generation, a uniformly random n-byte string S is sampled from a secure source of randomness. This seed S MUST NOT be confused with the public seed SEED. The seed S MUST be independent of SEED, and because it is the main secret, it MUST be kept secret. This seed S is used to generate an n-byte value S_ots for each WOTS+ key pair. The n-byte value S_ots can then be used to compute the respective WOTS+ private key using the method described in Section 3.1.7. The seeds for the WOTS+ key pairs are computed as S_ots[i] = PRF(S, toByte(i, 32)) where i is the index of the WOTS+ key pair. An advantage of this method is that a WOTS+ key can be computed using only len + 1 evaluations of PRF when S is given.
4.1.12. Free Index Handling and Partial Private Keys

Some applications might require working with partial private keys or copies of private keys. Examples include load balancing and delegation of signing rights or proxy signatures. Such applications MAY use their own key format and MAY use a signing algorithm different from the one described above. The index in partial private keys or copies of a private key MAY be manipulated as required by the applications. However, applications MUST establish means that guarantee that each index, and thereby each WOTS+ key pair, is used to sign only a single message.

4.2. XMSS^MT: Multi-Tree XMSS

XMSS^MT is a method for signing a large but fixed number of messages. It was first described in [HRB13]. It builds on XMSS. XMSS^MT uses a tree of several layers of XMSS trees, a so-called hypertree. The trees on top and intermediate layers are used to sign the root nodes of the trees on the respective layer below. Trees on the lowest layer are used to sign the actual messages. All XMSS trees have equal height.

Consider an XMSS^MT tree of total height \( h \) that has \( d \) layers of XMSS trees of height \( h / d \). Then, layer \( d - 1 \) contains one XMSS tree, layer \( d - 2 \) contains \( 2^{(h / d)} \) XMSS trees, and so on. Finally, layer 0 contains \( 2^{(h - h / d)} \) XMSS trees.

4.2.1. XMSS^MT Parameters

In addition to all XMSS parameters, an XMSS^MT system requires the number of tree layers \( d \), specified as an integer value that divides \( h \) without remainder. The same tree height \( h / d \) and the same Winternitz parameter \( w \) are used for all tree layers.

All the trees on higher layers sign root nodes of other trees, with the root nodes being \( n \)-byte strings. Hence, no message compression is needed, and WOTS+ is used to sign the root nodes themselves instead of their hash values.

4.2.2. XMSS^MT Key Generation

An XMSS^MT private key \( SK_{MT} \) (S for secret) consists of one reduced XMSS private key for each XMSS tree. These reduced XMSS private keys just contain the WOTS+ private keys corresponding to that XMSS key pair; they do not contain a pseudorandom function key, index, public seed, or root node. Instead, \( SK_{MT} \) contains a single \( n \)-byte pseudorandom function key \( SK_{PRF} \), a single \( \lceil h / 8 \rceil \)-byte index \( idx_{MT} \), a single \( n \)-byte seed \( SEED \), and a single root value \( root \).
(which is the root of the single tree on the top layer). The index is a global index over all WOTS+ key pairs of all XMSS trees on layer 0. It is initialized with 0. It stores the index of the last used WOTS+ key pair on the bottom layer, i.e., a number between 0 and 2^h - 1.

The reduced XMSS private keys MUST either be generated as described in Section 4.1.3 or be generated using a cryptographic pseudorandom method as discussed in Section 4.2.6. As for XMSS, the PRF key SK_PRF MUST be sampled from a secure source of randomness that follows the uniform distribution. SEED is generated as a uniformly random n-byte string. Although SEED is public, it is critical for security that it is generated using a good entropy source. The root is the root node of the single XMSS tree on the top layer. Its computation is explained below. As for XMSS, root and SEED are public information and would classically be considered part of the public key. However, as both are needed for signing, which only takes the private key, they are also part of SK_MT.

This document does not define any specific format for the XMSS^MT private key SK_MT as it is not required for interoperability. Algorithms 15 and 16 use a function getXMSS_SK(SK, x, y) that outputs the reduced private key of the x^th XMSS tree on the y^th layer.

The XMSS^MT public key PK_MT contains the root of the single XMSS tree on layer d - 1 and the seed SEED. These are the same values as in the private key SK_MT. The pseudorandom function PRF keyed with SEED is used to generate the bitmasks and keys for all XMSS trees. XMSSMT_keyGen (Algorithm 15) shows example pseudocode to generate SK_MT and PK_MT. The n-byte root node of the top-layer tree is computed using treeHash. The algorithm XMSSMT_keyGen outputs an XMSS^MT private key SK_MT and an XMSS^MT public key PK_MT. The algorithm below gives an example of how the reduced XMSS private keys can be generated. However, any of the above mentioned ways is acceptable as long as the cryptographic strength of the used method matches or supersedes that of the used XMSS^MT parameter set.
Algorithm 15: XMSSMT_keyGen - Generate an XMSS^MT key pair

Input: No input
Output: XMSS^MT private key SK_MT, XMSS^MT public key PK_MT

// Example initialization
idx_MT = 0;
setIdx(SK_MT, idx_MT);
initialize SK_PRF with a uniformly random n-byte string;
setSK_PRF(SK_MT, SK_PRF);
initialize SEED with a uniformly random n-byte string;
setSEED(SK_MT, SEED);

// Generate reduced XMSS private keys
ADRS = toByte(0, 32);
for ( layer = 0; layer < d; layer++ ) {
    ADRS.setLayerAddress(layer);
    for ( tree = 0; tree <
        (1 << ((d - 1 - layer) * (h / d)));
            tree++ ) {
        ADRS.setTreeAddress(tree);
        for ( i = 0; i < 2^(h / d); i++ ) {
            wots_sk[i] = WOTS_genSK();
        }
        setXMSS_SK(SK_MT, wots_sk, tree, layer);
    }
}

SK = getXMSS_SK(SK_MT, 0, d - 1);
setSEED(SK, SEED);
root = treeHash(SK, 0, h / d, ADRS);
setRoot(SK_MT, root);

PK_MT = OID || root || SEED;
return (SK_MT || PK_MT);

The above is just an example algorithm. It is strongly RECOMMENDED to use pseudorandom key generation to reduce the private key size. Public and private key generation MAY be interleaved to save space. In particular, when a pseudorandom method is used to generate the private key, generation MAY be delayed to the point that the respective WOTS+ key pair is needed by another algorithm.
The format of an XMSS^MT public key is given below.

XMSS^MT Public Key

4.2.3. XMSS^MT Signature

An XMSS^MT signature \( \text{Sig}_{\text{MT}} \) is a byte string of length \( \lceil \text{h} / 8 \rceil + n + (\text{h} + d \cdot \text{len}) \cdot n \). It consists of:

- the index \( \text{idx}_\text{sig} \) of the used WOTS+ key pair on the bottom layer (\( \lceil \text{h} / 8 \rceil \) bytes),
- a byte string \( r \) used for randomized message hashing (\( n \) bytes), and
- \( d \) reduced XMSS signatures (\( (\text{h} / d + \text{len}) \cdot n \) bytes each).

The reduced XMSS signatures only contain a WOTS+ signature \( \text{sig}_{\text{ots}} \) and an authentication path \( \text{auth} \). They contain no index \( \text{idx} \) and no byte string \( r \).
The data format for a signature is given below.

```
+---------------------------------+            
|                                 |            
+---------------------------------+            
|          index idx_sig          |   ceil(h / 8) bytes         
+---------------------------------+            
|          randomness r           |   n bytes         
+---------------------------------+            
|  (reduced) XMSS signature Sig  |   (h / d + len) * n bytes  
|      (bottom layer 0)          |            
+---------------------------------+            
|  (reduced) XMSS signature Sig  |   (h / d + len) * n bytes  
|      (layer 1)                 |            
+---------------------------------+            
   ....                           
+---------------------------------+            
|  (reduced) XMSS signature Sig  |   (h / d + len) * n bytes  
|      (layer d - 1)             |            
+---------------------------------+            
XMSS^MT Signature
```

4.2.4. XMSS^MT Signature Generation

To compute the XMSS^MT signature Sig_MT of a message M using an XMSS^MT private key SK_MT, XMSSMT_sign (Algorithm 16) described below uses treeSig as defined in Section 4.1.9. First, the signature index is set to idx_sig. Next, PRF is used to compute a pseudorandom n-byte string r. This n-byte string, idx_sig, and the root node from PK_MT are then used to compute a randomized message digest of length n. The message digest is signed using the WOTS+ key pair on the bottom layer with absolute index idx. The authentication path for the WOTS+ key pair and the root of the containing XMSS tree are computed. The root is signed by the parent XMSS tree. This is repeated until the top tree is reached.
Algorithm 16: XMSSMT_sign - Generate an XMSS^MT signature and update the XMSS^MT private key

Input: Message M, XMSS^MT private key SK_MT
Output: Updated SK_MT, signature Sig_MT

// Init
ADRS = toByte(0, 32);
SEED = getSEED(SK_MT);
SK_PRF = getSK_PRF(SK_MT);
idx_sig = getIdx(SK_MT);

// Update SK_MT
setIdx(SK_MT, idx_sig + 1);

// Message compression
byte[n] r = PRF(SK_PRF, toByte(idx_sig, 32));
byte[n] M' = H_msg(r || getRoot(SK_MT) || (toByte(idx_sig, n)), M);

// Sign
Sig_MT = idx_sig;
unsigned int idx_tree = (h - h / d) most significant bits of idx_sig;
unsigned int idx_leaf = (h / d) least significant bits of idx_sig;
SK = idx_leaf || getXMSS_SK(SK_MT, idx_tree, 0) || SK_PRF
    || toByte(0, n) || SEED;
ADRS.setLayerAddress(0);
ADRS.setTreeAddress(idx_tree);
Sig_tmp = treeSig(M', SK, idx_leaf, ADRS);
Sig_MT = Sig_MT || r || Sig_tmp;
for ( j = 1; j < d; j++ ) {
    root = treeHash(SK, 0, h / d, ADRS);
    idx_leaf = (h / d) least significant bits of idx_tree;
    idx_tree = (h - j * (h / d)) most significant bits of idx_tree;
    SK = idx_leaf || getXMSS_SK(SK_MT, idx_tree, j) || SK_PRF
        || toByte(0, n) || SEED;
    ADRS.setLayerAddress(j);
    ADRS.setTreeAddress(idx_tree);
    Sig_tmp = treeSig(root, SK, idx_leaf, ADRS);
    Sig_MT = Sig_MT || Sig_tmp;
}
return SK_MT || Sig_MT;
Algorithm 16 is only one method to compute XMSS^MT signatures. Time-memory trade-offs exist that allow reduction of the signing time to less than the signing time of an XMSS scheme with tree height $h / d$. These trade-offs 1) prevent certain values from being recomputed several times by keeping a state and 2) distribute all computations over all signature generations. Details can be found in [Huelsing13a].

4.2.5. XMSS^MT Signature Verification

XMSS^MT signature verification (Algorithm 17) can be summarized as $d$ XMSS signature verifications with small changes. First, the message is hashed. The XMSS signatures are then all on n-byte values. Second, instead of comparing the computed root node to a given value, a signature on this root node is verified. Only the root node of the top tree is compared to the value in the XMSS^MT public key. XMSSMT_verify uses XMSS_rootFromSig. The function getXMSSSignature(Sig_MT, i) returns the $i$th reduced XMSS signature from the XMSS^MT signature Sig_MT. XMSSMT_verify takes as input an XMSS^MT signature Sig_MT, a message $M$, and a public key PK_MT. XMSSMT_verify returns true if and only if Sig_MT is a valid signature on $M$ under public key PK_MT. Otherwise, it returns false.

Algorithm 17: XMSSMT_verify - Verify an XMSS^MT signature Sig_MT on a message $M$ using an XMSS^MT public key PK_MT

Input: XMSS^MT signature Sig_MT, message $M$, XMSS^MT public key PK_MT
Output: Boolean

idx_sig = getIdx(Sig_MT);
SEED = getSEED(PK_MT);
ADRS = toByte(0, 32);

byte[n] $M' = H_{msg}(getR(Sig_MT) \ || \ getRoot(PK_MT) \ || \ \text{toByte}(idx_sig, n)), M);

unsigned int idx_leaf
    = (h / d) least significant bits of idx_sig;
unsigned int idx_tree
    = (h - h / d) most significant bits of idx_sig;
Sig' = getXMSSSignature(Sig_MT, 0);
ADRS.setLayerAddress(0);
ADRS.setTreeAddress(idx_tree);
byte[n] node = XMSS_rootFromSig(idx_leaf, getSig_ots(Sig'),
    getAuth(Sig'), M', SEED, ADRS);
for ( j = 1; j < d; j++ ) {
    idx_leaf = (h / d) least significant bits of idx_tree;
    idx_tree = (h - j * h / d) most significant bits of idx_tree;
    Sig' = getXMSSSignature(Sig_MT, j);
    ADRS.setLayerAddress(j);
    ADRS.setTreeAddress(idx_tree);
    node = XMSS_rootFromSig(idx_leaf, getSig_ots(Sig'),
                           getAuth(Sig'), node, SEED, ADRS);
}
if ( node == getRoot(PK_MT) ) {
    return true;
} else {
    return false;
}

4.2.6. Pseudorandom Key Generation

Like for XMSS, an implementation MAY use a cryptographically secure pseudorandom method to generate the XMSS^MT private key from a single n-byte value. For example, the method explained below MAY be used. Other methods, such as the one in [HRS16], MAY be used. The choice of a pseudorandom method does not affect interoperability, but the cryptographic strength MUST match that of the used XMSS^MT parameters.

For XMSS^MT, a method similar to that for XMSS and WOTS+ can be used. The method uses PRF. During key generation, a uniformly random n-byte string S_MT is sampled from a secure source of randomness. This seed S_MT is used to generate one n-byte value S for each XMSS key pair. This n-byte value can be used to compute the respective XMSS private key using the method described in Section 4.1.11. Let S[x][y] be the seed for the x^th XMSS private key on layer y. The seeds are computed as S[x][y] = PRF(PRF(S, toByte(y, 32)), toByte(x, 32)).

4.2.7. Free Index Handling and Partial Private Keys

The content of Section 4.1.12 also applies to XMSS^MT.

5. Parameter Sets

This section provides basic parameter sets that are assumed to cover most relevant applications. Parameter sets for two classical security levels are defined. Parameters with n = 32 provide a classical security level of 256 bits. Parameters with n = 64 provide a classical security level of 512 bits. Considering quantum-computer-aided attacks, these output sizes yield post-quantum security of 128 and 256 bits, respectively.
While this document specifies several parameter sets, an implementation is only REQUIRED to provide support for verification of all REQUIRED parameter sets. The REQUIRED parameter sets all use SHA2-256 to instantiate all functions. The REQUIRED parameter sets are only distinguished by the tree height parameter $h$ (which determines the number of signatures that can be done with a single key pair) and the number of layers $d$ (which defines a trade-off between speed and signature size). An implementation MAY provide support for signature generation using any of the proposed parameter sets. For convenience, this document defines a default option for XMSS (XMSS_SHA2_20_256) and XMSS^MT (XMSSMT-SHA2_60/3_256). These are supposed to match the most generic requirements.

5.1. Implementing the Functions

For the $n = 32$ setting, we give parameters that use SHA2-256 as defined in [FIPS180] and other parameters that use the SHA3/Keccak-based extendable-output function SHAKE-128 as defined in [FIPS202]. For the $n = 64$ setting, we give parameters that use SHA2-512 as defined in [FIPS180] and other parameters that use the SHA3/Keccak-based extendable-output functions SHAKE-256 as defined in [FIPS202]. The parameter sets using SHA2-256 are mandatory for deployment and therefore MUST be provided by any implementation. The remaining parameter sets specified in this document are OPTIONAL.

SHA2 does not provide a keyed-mode itself. To implement the keyed hash functions, the following is used for SHA2 with $n = 32$:

- $F$: SHA2-256(toByte(0, 32) || KEY || M),
- $H$: SHA2-256(toByte(1, 32) || KEY || M),
- $H_{msg}$: SHA2-256(toByte(2, 32) || KEY || M), and
- $PRF$: SHA2-256(toByte(3, 32) || KEY || M).

Accordingly, for SHA2 with $n = 64$ we use:

- $F$: SHA2-512(toByte(0, 64) || KEY || M),
- $H$: SHA2-512(toByte(1, 64) || KEY || M),
- $H_{msg}$: SHA2-512(toByte(2, 64) || KEY || M), and
- $PRF$: SHA2-512(toByte(3, 64) || KEY || M).
The n-byte padding is used for two reasons. First, it is necessary that the internal compression function takes 2n-byte blocks, but keys are n and 3n bytes long. Second, the padding is used to achieve independence of the different function families. Finally, for the PRF, no full-fledged Hash-Based Message Authentication Code (HMAC) is needed as the message length is fixed, meaning that standard length extension attacks are not a concern here. For that reason, the simpler construction above suffices.

Similar constructions are used with SHA3. To implement the keyed hash functions, the following is used for SHA3 with n = 32:

\[
\begin{align*}
F & : \text{SHAKE128(toByte(0, 32) || KEY || M, 256)}, \\
H & : \text{SHAKE128(toByte(1, 32) || KEY || M, 256)}, \\
H_{\text{msg}} & : \text{SHAKE128(toByte(2, 32) || KEY || M, 256)}, \\
\text{PRF} & : \text{SHAKE128(toByte(3, 32) || KEY || M, 256)}.
\end{align*}
\]

Accordingly, for SHA3 with n = 64, we use:

\[
\begin{align*}
F & : \text{SHAKE256(toByte(0, 64) || KEY || M, 512)}, \\
H & : \text{SHAKE256(toByte(1, 64) || KEY || M, 512)}, \\
H_{\text{msg}} & : \text{SHAKE256(toByte(2, 64) || KEY || M, 512)}, \\
\text{PRF} & : \text{SHAKE256(toByte(3, 64) || KEY || M, 512)}.
\end{align*}
\]

As for SHA2, an initial n-byte identifier is used to achieve independence of the different function families. While a shorter identifier could be used in case of SHA3, we use n bytes for consistency with the SHA2 implementations.
5.2. WOTS+ Parameters

To fully describe a WOTS+ signature method, the parameters n and w, as well as the functions F and PRF, MUST be specified. The following table defines several WOTS+ signature systems, each of which is identified by a name. Naming follows this convention: WOTSP-[Hashfamily]_[n in bits]. Naming does not include w as all parameter sets in this document use w=16. Values for len are provided for convenience.

<table>
<thead>
<tr>
<th>Name</th>
<th>F / PRF</th>
<th>n</th>
<th>w</th>
<th>len</th>
</tr>
</thead>
<tbody>
<tr>
<td>REQUIRED:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WOTSP-SHA2_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
</tr>
<tr>
<td>OPTIONAL:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WOTSP-SHA2_512</td>
<td>SHA2-512</td>
<td>64</td>
<td>16</td>
<td>131</td>
</tr>
<tr>
<td>WOTSP-SHAKE_256</td>
<td>SHAKE128</td>
<td>32</td>
<td>16</td>
<td>67</td>
</tr>
<tr>
<td>WOTSP-SHAKE_512</td>
<td>SHAKE256</td>
<td>64</td>
<td>16</td>
<td>131</td>
</tr>
</tbody>
</table>

Table 1

The implementation of the single functions is done as described above. External Data Representation (XDR) formats for WOTS+ are listed in Appendix A.

5.3. XMSS Parameters

To fully describe an XMSS signature method, the parameters n, w, and h, as well as the functions F, H, H_msg, and PRF, MUST be specified. The following table defines different XMSS signature systems, each of which is identified by a name. Naming follows this convention: XMSS-[Hashfamily]_[h]_[n in bits]. Naming does not include w as all parameter sets in this document use w=16.
### Table 2

The XDR formats for XMSS are listed in Appendix B.

#### 5.3.1. Parameter Guide

In contrast to traditional signature schemes like RSA or Digital Signature Algorithm (DSA), XMSS has a tree height parameter h that determines the number of messages that can be signed with one key pair. Increasing the height allows using a key pair for more signatures, but it also increases the signature size and slows down key generation, signing, and verification. To demonstrate the impact of different values of h, the following table shows signature size and runtimes. Runtimes are given as the number of calls to F and H when the BDS algorithm is used to compute authentication paths for

<table>
<thead>
<tr>
<th>Name</th>
<th>Functions</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>REQUIRED:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XMSS-SHA2_10_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHA2_16_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHA2_20_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
</tr>
<tr>
<td>OPTIONAL:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XMSS-SHA2_10_512</td>
<td>SHA2-512</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHA2_16_512</td>
<td>SHA2-512</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHA2_20_512</td>
<td>SHA2-512</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>20</td>
</tr>
<tr>
<td>XMSS-SHAKE_10_256</td>
<td>SHAKE128</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHAKE_16_256</td>
<td>SHAKE128</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHAKE_20_256</td>
<td>SHAKE128</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
</tr>
<tr>
<td>XMSS-SHAKE_10_512</td>
<td>SHAKE256</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHAKE_16_512</td>
<td>SHAKE256</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHAKE_20_512</td>
<td>SHAKE256</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>20</td>
</tr>
</tbody>
</table>
the worst case. The last column shows the number of messages that can be signed with one key pair. The numbers are the same for the XMSS-SHAKE instances with same parameters h and n.

<table>
<thead>
<tr>
<th>Name</th>
<th>Sig</th>
<th>KeyGen</th>
<th>Sign</th>
<th>Verify</th>
<th>#Sigs</th>
</tr>
</thead>
<tbody>
<tr>
<td>REQUIRED:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XMSS-SHA2_10_256</td>
<td>2,500</td>
<td>1,238,016</td>
<td>5,725</td>
<td>1,149</td>
<td>2^10</td>
</tr>
<tr>
<td>XMSS-SHA2_16_256</td>
<td>2,692</td>
<td>79*10^6</td>
<td>9,163</td>
<td>1,155</td>
<td>2^16</td>
</tr>
<tr>
<td>XMSS-SHA2_20_256</td>
<td>2,820</td>
<td>1,268*10^6</td>
<td>11,455</td>
<td>1,159</td>
<td>2^20</td>
</tr>
<tr>
<td>OPTIONAL:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XMSS-SHA2_10_512</td>
<td>9,092</td>
<td>2,417,664</td>
<td>11,165</td>
<td>2,237</td>
<td>2^10</td>
</tr>
<tr>
<td>XMSS-SHA2_16_512</td>
<td>9,476</td>
<td>155*10^6</td>
<td>17,867</td>
<td>2,243</td>
<td>2^16</td>
</tr>
<tr>
<td>XMSS-SHA2_20_512</td>
<td>9,732</td>
<td>2,476*10^6</td>
<td>22,335</td>
<td>2,247</td>
<td>2^20</td>
</tr>
</tbody>
</table>

Table 3

As a default, users without special requirements should use option XMSS-SHA2_20_256, which allows signing of 2^20 messages with one key pair and provides reasonable speed and signature size. Users that require more signatures per key pair or faster key generation should consider XMSS^MT.

5.4. XMSS^MT Parameters

To fully describe an XMSS^MT signature method, the parameters n, w, h, and d, as well as the functions F, H, H_msg, and PRF, MUST be specified. The following table defines different XMSS^MT signature systems, each of which is identified by a name. Naming follows this convention: XMSSMT-[Hashfamily]_[h]/[d]_[n in bits]. Naming does not include w as all parameter sets in this document use w=16.
<table>
<thead>
<tr>
<th>Name</th>
<th>Functions</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>REQUIRED:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XMSSMT-SHA2_20/2_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_20/4_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/2_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/4_256</td>
<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>4</td>
</tr>
<tr>
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<td>SHA2-256</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>8</td>
</tr>
<tr>
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<td>67</td>
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<tr>
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<td>67</td>
<td>60</td>
<td>6</td>
</tr>
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<td>67</td>
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<td>12</td>
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<td></td>
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<tr>
<td>XMSSMT-SHA2_20/2_512</td>
<td>SHA2-512</td>
<td>64</td>
<td>16</td>
<td>131</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_20/4_512</td>
<td>SHA2-512</td>
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<td>131</td>
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<tr>
<td>XMSSMT-SHA2_40/2_512</td>
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<td>131</td>
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<td>2</td>
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<tr>
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<td>131</td>
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<tr>
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<td>60</td>
<td>12</td>
</tr>
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<td>16</td>
<td>67</td>
<td>20</td>
<td>2</td>
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<tr>
<td>XMSSMT-SHAKE_20/4_256</td>
<td>SHAKE128</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHAKE_40/2_256</td>
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<td>16</td>
<td>67</td>
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<td>16</td>
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<td>4</td>
</tr>
<tr>
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<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>8</td>
</tr>
</tbody>
</table>
Table 4

XDR formats for XMSS^MT are listed in Appendix C.

5.4.1. Parameter Guide

In addition to the tree height parameter already used for XMSS, XMSS^MT has the parameter d that determines the number of tree layers. XMSS can be understood as XMSS^MT with a single layer, i.e., d=1. Hence, the choice of h has the same effect as for XMSS. The number of tree layers provides a trade-off between signature size on the one side and key generation and signing speed on the other side. Increasing the number of layers reduces key generation time exponentially and signing time linearly at the cost of increasing the signature size linearly. Essentially, an XMSS^MT signature contains one WOTSP signature per layer. Speed roughly corresponds to d-times the speed for XMSS with trees of height h/d.

To demonstrate the impact of different values of h and d, the following table shows signature size and runtimes. Runtimes are given as the number of calls to F and H when the BDS algorithm and distributed signature generation are used. Timings are worst-case times. The last column shows the number of messages that can be signed with one key pair. The numbers are the same for the XMSS-
SHAKE instances with same parameters $h$ and $n$. Due to formatting limitations, only the parameter part of the parameter set names are given, omitting the name "XMSSMT".

<table>
<thead>
<tr>
<th>Name</th>
<th>Sig</th>
<th>KeyGen</th>
<th>Sign</th>
<th>Verify</th>
<th>#Sigs</th>
</tr>
</thead>
<tbody>
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<td>REQUIRED:</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SHA2_20/2_256</td>
<td>4,963</td>
<td>2,476,032</td>
<td>7,227</td>
<td>2,298</td>
<td>$2^{20}$</td>
</tr>
<tr>
<td>SHA2_20/4_256</td>
<td>9,251</td>
<td>154,752</td>
<td>4,170</td>
<td>4,576</td>
<td>$2^{20}$</td>
</tr>
<tr>
<td>SHA2_40/2_256</td>
<td>5,605</td>
<td>2,535*10^6</td>
<td>13,417</td>
<td>2,318</td>
<td>$2^{40}$</td>
</tr>
<tr>
<td>SHA2_40/4_256</td>
<td>9,893</td>
<td>4,952,064</td>
<td>7,227</td>
<td>4,596</td>
<td>$2^{40}$</td>
</tr>
<tr>
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<td>309,504</td>
<td>4,170</td>
<td>9,152</td>
<td>$2^{40}$</td>
</tr>
<tr>
<td>SHA2_60/3_256</td>
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<td>3,803*10^6</td>
<td>13,417</td>
<td>3,477</td>
<td>$2^{60}$</td>
</tr>
<tr>
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<td>7,227</td>
<td>6,894</td>
<td>$2^{60}$</td>
</tr>
<tr>
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<tr>
<td>OPTIONAL:</td>
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<td></td>
<td></td>
</tr>
<tr>
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<td>18,115</td>
<td>4,835,328</td>
<td>14,075</td>
<td>4,474</td>
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</tr>
<tr>
<td>SHA2_20/4_512</td>
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<td>302,208</td>
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<td>8,928</td>
<td>$2^{20}$</td>
</tr>
<tr>
<td>SHA2_40/2_512</td>
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<td>4,494</td>
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<td>36,165</td>
<td>9,670,656</td>
<td>14,075</td>
<td>8,948</td>
<td>$2^{40}$</td>
</tr>
<tr>
<td>SHA2_40/8_512</td>
<td>69,701</td>
<td>604,416</td>
<td>8,138</td>
<td>17,856</td>
<td>$2^{40}$</td>
</tr>
<tr>
<td>SHA2_60/3_512</td>
<td>29,064</td>
<td>7,427*10^6</td>
<td>26,025</td>
<td>6,741</td>
<td>$2^{60}$</td>
</tr>
<tr>
<td>SHA2_60/6_512</td>
<td>54,216</td>
<td>14,505,984</td>
<td>14,075</td>
<td>13,422</td>
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</tr>
<tr>
<td>SHA2_60/12_512</td>
<td>104,520</td>
<td>906,624</td>
<td>8,138</td>
<td>26,784</td>
<td>$2^{60}$</td>
</tr>
</tbody>
</table>

Table 5
As a default, users without special requirements should use option XMSSMT-SHA2_60/3_256, which allows signing of $2^{60}$ messages with one key pair (this is a virtually unbounded number of signatures). At the same time, signature size and speed are well balanced.

6. Rationale

The goal of this note is to describe the WOTS+, XMSS, and XMSS^MT algorithms based on the scientific literature. The description is done in a modular way that allows basing a description of stateless hash-based signature algorithms like SPHINCS [BHH15] on it.

This note slightly deviates from the scientific literature by using a tweak that prevents multi-user and multi-target attacks against $H_{msg}$. To this end, the public key as well as the index of the used one-time key pair become part of the hash function key. Thereby, we achieve a domain separation that forces an attacker to decide which hash value to attack.

For the generation of the randomness used for randomized message hashing, we apply a PRF, keyed with a secret value, to the index of the used one-time key pair instead of the message. The reason is that this requires processing the message only once instead of twice. For long messages, this improves speed and simplifies implementations on resource-constrained devices that cannot hold the entire message in storage.

We give one mandatory set of parameters using SHA2-256. The reasons are twofold. On the one hand, SHA2-256 is part of most cryptographic libraries. On the other hand, a 256-bit hash function leads to parameters that provide 128 bits of security even against quantum-computer-aided attacks. A post-quantum security level of 256 bits seems overly conservative. However, to prepare for possible cryptanalytic breakthroughs, we also provide OPTIONAL parameter sets using the less widely supported SHA2-512, SHAKE-256, and SHAKE-512 functions.

We suggest the value $w = 16$ for the Winternitz parameter. No bigger values are included since the decrease in signature size then becomes less significant. Furthermore, the value $w = 16$ considerably simplifies the implementations of some of the algorithms. Please note that we do allow $w = 4$ but limit the specified parameter sets to $w = 16$ for efficiency reasons.
The signature and public key formats are designed so that they are easy to parse. Each format starts with a 32-bit enumeration value that indicates all of the details of the signature algorithm and hence defines all of the information that is needed in order to parse the format.

7. Reference Code

For testing purposes, a reference implementation in C is available. The code contains a basic implementation that closely follows the pseudocode in this document and an optimized implementation that uses the BDS algorithm [BDS08] to compute authentication paths and distributed signature generation as described in [HRB13] for XMSS^MT.

The code is permanently available at <https://github.com/joostrijneveld/xmss-reference>.

8. IANA Considerations

The Internet Assigned Numbers Authority (IANA) has created three registries: one for WOTS+ signatures (as defined in Section 3), one for XMSS signatures (as defined in Section 4), and one for XMSS^MT signatures (as defined in Section 4). For the sake of clarity and convenience, the first collection of WOTS+, XMSS, and XMSS^MT parameter sets is defined in Section 5. Additions to these registries require that a specification be documented in an RFC or another permanent and readily available reference in sufficient detail as defined by the "Specification Required" policy described in [RFC8126] to make interoperability between independent implementations possible. Each entry in these registries contains the following elements:

- a short name, such as "XMSS_SHA2_20_256",
- a positive number, and
- a reference to a specification that completely defines the signature method test cases or provides a reference implementation that can be used to verify the correctness of an implementation (or a reference to such an implementation).

Requests to add an entry to these registries MUST include the name and the reference. The number is assigned by IANA. These number assignments SHOULD use the smallest available positive number. Submitters MUST have their requests reviewed and approved. Designated Experts for this task as requested by the "Specification Required" policy defined by [RFC8126] will be assigned by the
Internet Engineering Steering Group (IESG). The IESG can be contacted at iesg@ietf.org. Interested applicants that are unfamiliar with IANA processes should visit <http://www.iana.org>.

The number 0x00000000 (decimal 0) is Reserved. The numbers between 0xDDDDDDDDD (decimal 3,722,304,989) and 0xFFFFFFFF (decimal 4,294,967,295) inclusive will not be assigned by IANA and are Reserved for Private Use; no attempt will be made to prevent multiple sites from using the same value in different (and incompatible) ways [RFC8126].

The "WOTS+ Signatures" registry is as follows.

<table>
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<td>this RFC</td>
</tr>
<tr>
<td>0x00000001</td>
<td>WOTSP-SHA2_256</td>
<td>Section 5.2</td>
</tr>
<tr>
<td>0x00000002</td>
<td>WOTSP-SHA2_512</td>
<td>Section 5.2</td>
</tr>
<tr>
<td>0x00000003</td>
<td>WOTSP-SHAKE_256</td>
<td>Section 5.2</td>
</tr>
<tr>
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<td>Section 5.2</td>
</tr>
</tbody>
</table>

Table 6
The "XMSS Signatures" registry is as follows.

<table>
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<td>this RFC</td>
</tr>
<tr>
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</tr>
<tr>
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<td>Section 5.3</td>
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<td>XMSS-SHAKE_16_256</td>
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</tr>
<tr>
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</tr>
<tr>
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<td>Section 5.3</td>
</tr>
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<td>Section 5.3</td>
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Table 7
The "XMSS^MT Signatures" registry is as follows.

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<th>Reference</th>
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</thead>
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<td>Reserved</td>
<td>this RFC</td>
</tr>
<tr>
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<td>Section 5.4</td>
</tr>
<tr>
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<td>XMSSMT-SHA2_20/4_256</td>
<td>Section 5.4</td>
</tr>
<tr>
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<td>XMSSMT-SHA2_40/2_256</td>
<td>Section 5.4</td>
</tr>
<tr>
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</tr>
<tr>
<td>0x00000007</td>
<td>XMSSMT-SHA2_60/6_256</td>
<td>Section 5.4</td>
</tr>
<tr>
<td>0x00000008</td>
<td>XMSSMT-SHA2_60/12_256</td>
<td>Section 5.4</td>
</tr>
<tr>
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<td>XMSSMT-SHA2_20/2_512</td>
<td>Section 5.4</td>
</tr>
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<td>XMSSMT-SHA2_20/4_512</td>
<td>Section 5.4</td>
</tr>
<tr>
<td>0x0000000B</td>
<td>XMSSMT-SHA2_40/2_512</td>
<td>Section 5.4</td>
</tr>
<tr>
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<td>XMSSMT-SHA2_40/4_512</td>
<td>Section 5.4</td>
</tr>
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<td>Section 5.4</td>
</tr>
<tr>
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</tr>
<tr>
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<td>Section 5.4</td>
</tr>
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<td>Section 5.4</td>
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<td>Section 5.4</td>
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<td>XMSSMT-SHAKE_40/4_256</td>
<td>Section 5.4</td>
</tr>
<tr>
<td>0x00000015</td>
<td>XMSSMT-SHAKE_40/8_256</td>
<td>Section 5.4</td>
</tr>
</tbody>
</table>
An IANA registration of a signature system does not constitute an endorsement of that system or its security.

9. Security Considerations

A signature system is considered secure if it prevents an attacker from forging a valid signature. More specifically, consider a setting in which an attacker gets a public key and can learn signatures on arbitrary messages of its choice. A signature system is secure if, even in this setting, the attacker cannot produce a new message/signature pair of his choosing such that the verification algorithm accepts.

Preventing an attacker from mounting an attack means that the attack is computationally too expensive to be carried out. There are various estimates for when a computation is too expensive to be done. For that reason, this note only describes how expensive it is for an attacker to generate a forgery. Parameters are accompanied by a bit security value. The meaning of bit security is as follows. A parameter set grants $b$ bits of security if the best attack takes at least $2^{(b - 1)}$ bit operations to achieve a success probability of...
1/2. Hence, to mount a successful attack, an attacker needs to perform \(2^b\) bit operations on average. The given values for bit security were estimated according to [HRS16].

9.1. Security Proofs

A full security proof for all schemes described in this document can be found in [HRS16]. This proof shows that an attacker has to break at least one out of certain security properties of the used hash functions and PRFs to forge a signature in any of the described schemes. The proof in [HRS16] considers an initial message compression different from the randomized hashing used here. We comment on this below. For the original schemes, these proofs show that an attacker has to break certain minimal security properties. In particular, it is not sufficient to break the collision resistance of the hash functions to generate a forgery.

More specifically, the requirements on the used functions are that \(F\) and \(H\) are post-quantum multi-function multi-target second-preimage resistant keyed functions, \(F\) fulfills an additional statistical requirement that roughly says that most images have at least two preimages, \(PRF\) is a post-quantum pseudorandom function, and \(H_{msg}\) is a post-quantum multi-target extended target collision-resistant keyed hash function. For detailed definitions of these properties see [HRS16]. To give some intuition: multi-function multi-target second-preimage resistance is an extension of second-preimage resistance to keyed hash functions, covering the case where an adversary succeeds if it finds a second preimage for one out of many values. The same holds for multi-target extended target collision resistance, which just lacks the multi-function identifier as target collision resistance already considers keyed hash functions. The proof in [HRS16] splits \(PRF\) into two functions. When \(PRF\) is used for pseudorandom key generation or generation of randomness for randomized message hashing, it is still considered a pseudorandom function. Whenever \(PRF\) is used to generate bitmasks and hash function keys, it is modeled as a random oracle. This is due to technical reasons in the proof, and an implementation using a pseudorandom function is secure.

The proof in [HRS16] considers classical randomized hashing for the initial message compression, i.e., \(H(r, M)\) instead of \(H(r \| \text{getRoot}(PK) \| \text{index}, M)\). This classical randomized hashing allows getting a security reduction from extended target collision resistance [HRS16], a property that is conjectured to be strictly weaker than collision resistance. However, it turns out that in this case, an attacker could still launch a multi-target attack even against multiple users at the same time. The reason is that the adversary attacking \(u\) users at the same time learns \(u \times 2^h\)
randomized hashes H(r_i_j || M_i_j) with signature index i in [0, 2^h - 1] and user index j in [0, u]. It suffices to find a single pair (r*, M*) such that H(r* || M*) = H(r_i_u || M_i_u) for one out of the u * 2^h learned hashes. Hence, an attacker can do a brute-force search in time 2^n / u * 2^h instead of 2^n.

The indexed randomized hashing H(r || getRoot(PK) || toByte(idx, n), M) used in this work makes the hash function calls position- and user-dependent. This thwarts the above attack because each hash function evaluation during an attack can only target one of the learned randomized hash values. More specifically, an attacker now has to decide which index idx and which root value to use for each query. If one assumes that the used hash function is a random function, it can be shown that a multi-user existential forgery attack that targets this message compression has a complexity of 2^n hash function calls.

The given bit security values were estimated based on the complexity of the best-known generic attacks against the required security properties of the used hash and pseudorandom functions, assuming conventional and quantum adversaries. At the time of writing, generic attacks are the best-known attacks for the parameters suggested in the classical setting. Also, in the quantum setting, there are no dedicated attacks known that perform better than generic attacks. Nevertheless, the topic of quantum cryptanalysis of hash functions is not as well understood as in the classical setting.

9.2. Minimal Security Assumptions

The assumptions one has to make to prove security of the described schemes are minimal in the following sense. Any signature algorithm that allows arbitrary size messages relies on the security of a cryptographic hash function, either on collision resistance or on extended target collision resistance if randomized hashing is used for message compression. For the schemes described here, this is already sufficient to be secure. In contrast, common signature schemes like RSA, DSA, and Elliptic Curve Digital Signature Algorithm (ECDSA) additionally rely on the conjectured hardness of certain mathematical problems.

9.3. Post-Quantum Security

A post-quantum cryptosystem is a system that is secure against attackers with access to a reasonably sized quantum computer. At the time of writing this note, whether or not it is feasible to build such a machine is an open conjecture. However, significant progress was made over the last few years in this regard. Hence, we consider it a matter of risk assessment to prepare for this case.
In contrast to RSA, DSA, and ECDSA, the described signature systems are post-quantum-secure if they are used with an appropriate cryptographic hash function. In particular, for post-quantum security, the size of n must be twice the size required for classical security. This is in order to protect against quantum square-root attacks due to Grover’s algorithm. [HRS16] shows that variants of Grover’s algorithm are the optimal generic attacks against the security properties of hash functions required for the described schemes.

As stated above, we only consider generic attacks here, as cryptographic hash functions should be deprecated as soon as dedicated attacks that perform significantly better exist. This also applies to the quantum setting. As soon as dedicated quantum attacks against the used hash function that can perform significantly better than the described generic attacks exist, these hash functions should not be used anymore for the described schemes, or the computation of the security level has to be redone.

10. References

10.1. Normative References


10.2. Informative References


Appendix A. WOTS+ XDR Formats

The WOTS+ signature and public key formats are formally defined using XDR [RFC4506] in order to provide an unambiguous, machine readable definition. Though XDR is used, these formats are simple and easy to parse without any special tools. Note that this representation includes all optional parameter sets. The same applies for the XMSS and XMSS\(^\text{MT}\) formats below.

A.1. WOTS+ Parameter Sets

WOTS+ parameter sets are defined using XDR syntax as follows:

/* ots_algorithm_type identifies a particular signature algorithm */

enum ots_algorithm_type {
    wotsp_reserved = 0x00000000,
    wotsp-sha2_256 = 0x00000001,
    wotsp-sha2_512 = 0x00000002,
    wotsp-shake_256 = 0x00000003,
    wotsp-shake_512 = 0x00000004,
};

A.2. WOTS+ Signatures

WOTS+ signatures are defined using XDR syntax as follows:

/* Byte strings */

typedef opaque bytestring32[32];
typedef opaque bytestring64[64];

union ots_signature switch (ots_algorithm_type type) {
    case wotsp-sha2_256:
    case wotsp-shake_256:
        bytestring32 ots_sig_n32_len67[67];
    case wotsp-sha2_512:
    case wotsp-shake_512:
        bytestring64 ots_sig_n64_len18[131];
    default:
        void; /* error condition */
};
A.3. WOTS+ Public Keys

WOTS+ public keys are defined using XDR syntax as follows:

```c
union ots_pubkey switch (ots_algorithm_type type) {
  case wotsp-sha2_256:
  case wotsp-shake_256:
    bytestring32 ots_pubk_n32_len67[67];
  case wotsp-sha2_512:
  case wotsp-shake_512:
    bytestring64 ots_pubk_n64_len18[131];
  default:
    void; /* error condition */
};
```

Appendix B. XMSS XDR Formats

B.1. XMSS Parameter Sets

XMSS parameter sets are defined using XDR syntax as follows:

```c
/* Byte strings */
typedef opaque bytestring4[4];

/* Definition of parameter sets */
enum xmss_algorithm_type {
  xmss_reserved = 0x00000000,
  /* 256 bit classical security, 128 bit post-quantum security */
  xmss-sha2_10_256 = 0x00000001,
  xmss-sha2_16_256 = 0x00000002,
  xmss-sha2_20_256 = 0x00000003,
  /* 512 bit classical security, 256 bit post-quantum security */
  xmss-sha2_10_512 = 0x00000004,
  xmss-sha2_16_512 = 0x00000005,
  xmss-sha2_20_512 = 0x00000006,
};
```
B.2. XMSS Signatures

XMSS signatures are defined using XDR syntax as follows:

```c
/* Authentication path types */
union xmss_path switch (xmss_algorithm_type type) {
    case xmss-sha2_10_256:
        case xmss-shake_10_256:
        bytestring32 path_n32_t10[10];

    case xmss-sha2_16_256:
        case xmss-shake_16_256:
        bytestring32 path_n32_t16[16];

    case xmss-sha2_20_256:
        case xmss-shake_20_256:
        bytestring32 path_n32_t20[20];

    case xmss-sha2_10_512:
        case xmss-shake_10_512:
        bytestring64 path_n64_t10[10];

    case xmss-sha2_16_512:
        case xmss-shake_16_512:
        bytestring64 path_n64_t16[16];

    case xmss-sha2_20_512:
        case xmss-shake_20_512:
        bytestring64 path_n64_t20[20];

    default:
        void;     /* error condition */
};
```
/* Types for XMSS random strings */

union random_string_xmss switch (xmss_algorithm_type type) {
    case xmss-sha2_10_256: 
    case xmss-sha2_16_256: 
    case xmss-sha2_20_256: 
    case xmss-shake_10_256: 
    case xmss-shake_16_256: 
    case xmss-shake_20_256: 
        bytestring32 rand_n32;
    case xmss-sha2_10_512: 
    case xmss-sha2_16_512: 
    case xmss-sha2_20_512: 
    case xmss-shake_10_512: 
    case xmss-shake_16_512: 
    case xmss-shake_20_512: 
        bytestring64 rand_n64;
    default: 
        void;     /* error condition */
};

/* Corresponding WOTS+ type for given XMSS type */

union xmss_ots_signature switch (xmss_algorithm_type type) {
    case xmss-sha2_10_256: 
    case xmss-sha2_16_256: 
    case xmss-sha2_20_256: 
        wotsp-sha2_256;
    case xmss-sha2_10_512: 
    case xmss-sha2_16_512: 
    case xmss-sha2_20_512: 
        wotsp-sha2_512;
    case xmss-shake_10_256: 
    case xmss-shake_16_256: 
    case xmss-shake_20_256: 
        wotsp-shake_256;
    case xmss-shake_10_512: 
    case xmss-shake_16_512: 
    case xmss-shake_20_512: 
        wotsp-shake_512;
default:
    void; /* error condition */
};

/* XMSS signature structure */

struct xmss_signature {
    /* WOTS+ key pair index */
    bytestring4 idx_sig;
    /* Random string for randomized hashing */
    random_string_xmss rand_string;
    /* WOTS+ signature */
    xmss_ots_signature sig_ots;
    /* authentication path */
    xmss_path nodes;
};

B.3. XMSS Public Keys

XMSS public keys are defined using XDR syntax as follows:

/* Types for bitmask seed */

union seed_switch (xmss_algorithm_type type) {
    case xmss-sha2_10_256:
    case xmss-sha2_16_256:
    case xmss-sha2_20_256:
    case xmss-shake_10_256:
    case xmss-shake_16_256:
    case xmss-shake_20_256:
        bytestring32 seed_n32;
    case xmss-sha2_10_512:
    case xmss-sha2_16_512:
    case xmss-sha2_20_512:
    case xmss-shake_10_512:
    case xmss-shake_16_512:
    case xmss-shake_20_512:
        bytestring64 seed_n64;
    default:
        void; /* error condition */
};
/ * Types for XMSS root node */

union xmss_root switch (xmss_algorithm_type type) {
    case xmss-sha2_10_256:
    case xmss-sha2_16_256:
    case xmss-sha2_20_256:
    case xmss-shake_10_256:
    case xmss-shake_16_256:
    case xmss-shake_20_256:
        bytestring32 root_n32;
    case xmss-sha2_10_512:
    case xmss-sha2_16_512:
    case xmss-sha2_20_512:
    case xmss-shake_10_512:
    case xmss-shake_16_512:
    case xmss-shake_20_512:
        bytestring64 root_n64;
    default:
        void; /* error condition */
};

/* XMSS public key structure */

struct xmss_public_key {
    xmss_root root; /* Root node */
    seed SEED; /* Seed for bitmasks */
};

Appendix C. XMSS^MT XDR Formats

C.1. XMSS^MT Parameter Sets

XMSS^MT parameter sets are defined using XDR syntax as follows:

/* Byte strings */

typedef opaque bytestring3[3];
typedef opaque bytestring5[5];
typedef opaque bytestring8[8];

/* Definition of parameter sets */

enum xmssmt_algorithm_type {
    xmssmt_reserved     = 0x00000000,
/* 256 bit classical security, 128 bit post-quantum security */

xmssmt-sha2_20/2_256 = 0x00000001,
xmssmt-sha2_20/4_256 = 0x00000002,
xmssmt-sha2_40/2_256 = 0x00000003,
xmssmt-sha2_40/4_256 = 0x00000004,
xmssmt-sha2_40/8_256 = 0x00000005,
xmssmt-sha2_60/3_256 = 0x00000006,
xmssmt-sha2_60/6_256 = 0x00000007,
xmssmt-sha2_60/12_256 = 0x00000008,

/* 512 bit classical security, 256 bit post-quantum security */

xmssmt-sha2_20/2_512 = 0x00000009,
xmssmt-sha2_20/4_512 = 0x0000000A,
xmssmt-sha2_40/2_512 = 0x0000000B,
xmssmt-sha2_40/4_512 = 0x0000000C,
xmssmt-sha2_40/8_512 = 0x0000000D,
xmssmt-sha2_60/3_512 = 0x0000000E,
xmssmt-sha2_60/6_512 = 0x0000000F,
xmssmt-sha2_60/12_512 = 0x00000010,

/* 256 bit classical security, 128 bit post-quantum security */

xmssmt-shake_20/2_256 = 0x00000011,
xmssmt-shake_20/4_256 = 0x00000012,
xmssmt-shake_40/2_256 = 0x00000013,
xmssmt-shake_40/4_256 = 0x00000014,
xmssmt-shake_40/8_256 = 0x00000015,
xmssmt-shake_60/3_256 = 0x00000016,
xmssmt-shake_60/6_256 = 0x00000017,
xmssmt-shake_60/12_256 = 0x00000018,

/* 512 bit classical security, 256 bit post-quantum security */

xmssmt-shake_20/2_512 = 0x00000019,
xmssmt-shake_20/4_512 = 0x0000001A,
xmssmt-shake_40/2_512 = 0x0000001B,
xmssmt-shake_40/4_512 = 0x0000001C,
xmssmt-shake_40/8_512 = 0x0000001D,
xmssmt-shake_60/3_512 = 0x0000001E,
xmssmt-shake_60/6_512 = 0x0000001F,
xmssmt-shake_60/12_512 = 0x00000020,
C.2. XMSS\(^{MT}\) Signatures

XMSS\(^{MT}\) signatures are defined using XDR syntax as follows:

```c
/* Type for XMSS\(^{MT}\) key pair index */
/* Depends solely on h */

union idx_sig_xmssmt switch (xmss_algorithm_type type) {
    case xmssmt-sha2_20/2_256:
    case xmssmt-sha2_20/4_256:
    case xmssmt-sha2_20/2_512:
    case xmssmt-sha2_20/4_512:
    case xmssmt-shake_20/2_256:
    case xmssmt-shake_20/4_256:
    case xmssmt-shake_20/2_512:
    case xmssmt-shake_20/4_512:
        bytestring3 idx3;
    case xmssmt-sha2_40/2_256:
    case xmssmt-sha2_40/4_256:
    case xmssmt-sha2_40/8_256:
    case xmssmt-sha2_40/2_512:
    case xmssmt-sha2_40/4_512:
    case xmssmt-sha2_40/8_512:
    case xmssmt-shape_40/2_256:
    case xmssmt-shape_40/4_256:
    case xmssmt-shape_40/8_256:
    case xmssmt-shape_40/2_512:
    case xmssmt-shape_40/4_512:
    case xmssmt-shape_40/8_512:
        bytestring5 idx5;
    case xmssmt-sha2_60/3_256:
    case xmssmt-sha2_60/6_256:
    case xmssmt-sha2_60/12_256:
    case xmssmt-sha2_60/3_512:
    case xmssmt-sha2_60/6_512:
    case xmssmt-sha2_60/12_512:
    case xmssmt-shape_60/3_256:
    case xmssmt-shape_60/6_256:
    case xmssmt-shape_60/12_256:
    case xmssmt-shape_60/3_512:
    case xmssmt-shape_60/6_512:
    case xmssmt-shape_60/12_512:
        bytestring8 idx8;
```

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default:
    void;  /* error condition */
};

union random_string_xmssmt switch (xmssmt_algorithm_type type) {
    case xmssmt-sha2_20/2_256:
    case xmssmt-sha2_20/4_256:
    case xmssmt-sha2_40/2_256:
    case xmssmt-sha2_40/4_256:
    case xmssmt-sha2_40/8_256:
    case xmssmt-sha2_60/3_256:
    case xmssmt-sha2_60/6_256:
    case xmssmt-sha2_60/12_256:
    case xmssmt-shake_20/2_256:
    case xmssmt-shake_20/4_256:
    case xmssmt-shake_40/2_256:
    case xmssmt-shake_40/4_256:
    case xmssmt-shake_40/8_256:
    case xmssmt-shake_60/3_256:
    case xmssmt-shake_60/6_256:
    case xmssmt-shake_60/12_256:
        bytestring32 rand_n32;
    case xmssmt-sha2_20/2_512:
    case xmssmt-sha2_20/4_512:
    case xmssmt-sha2_40/2_512:
    case xmssmt-sha2_40/4_512:
    case xmssmt-sha2_40/8_512:
    case xmssmt-sha2_60/3_512:
    case xmssmt-sha2_60/6_512:
    case xmssmt-sha2_60/12_512:
    case xmssmt-shake_20/2_512:
    case xmssmt-shake_20/4_512:
    case xmssmt-shake_40/2_512:
    case xmssmt-shake_40/4_512:
    case xmssmt-shake_40/8_512:
    case xmssmt-shake_60/3_512:
    case xmssmt-shake_60/6_512:
    case xmssmt-shake_60/12_512:
        bytestring64 rand_n64;
    default:
        void;  /* error condition */
};

/* Type for reduced XMSS signatures */
union xmss_reduced (xmss_algorithm_type type) {
    case xmssmt-sha2_20/2_256:
    case xmssmt-sha2_40/4_256:
    case xmssmt-sha2_60/6_256:
    case xmssmt-shake_20/2_256:
    case xmssmt-shake_40/4_256:
    case xmssmt-shake_60/6_256:
        bytestring32 xmss_reduced_n32_t77[77];
    case xmssmt-sha2_20/4_256:
    case xmssmt-sha2_40/8_256:
    case xmssmt-sha2_60/12_256:
    case xmssmt-shake_20/4_256:
    case xmssmt-shake_40/8_256:
    case xmssmt-shake_60/12_256:
        bytestring32 xmss_reduced_n32_t72[72];
    case xmssmt-sha2_40/2_256:
    case xmssmt-sha2_60/3_256:
    case xmssmt-shake_40/2_256:
    case xmssmt-shake_60/3_256:
        bytestring32 xmss_reduced_n32_t87[87];
    case xmssmt-sha2_20/2_512:
    case xmssmt-sha2_40/4_512:
    case xmssmt-sha2_60/6_512:
    case xmssmt-shake_20/2_512:
    case xmssmt-shake_40/4_512:
    case xmssmt-shake_60/6_512:
        bytestring64 xmss_reduced_n32_t141[141];
    case xmssmt-sha2_20/4_512:
    case xmssmt-sha2_40/8_512:
    case xmssmt-sha2_60/12_512:
    case xmssmt-shake_20/4_512:
    case xmssmt-shake_40/8_512:
    case xmssmt-shake_60/12_512:
        bytestring64 xmss_reduced_n32_t136[136];
    case xmssmt-sha2_40/2_512:
    case xmssmt-sha2_60/3_512:
    case xmssmt-shake_40/2_512:
    case xmssmt-shake_60/3_512:
        bytestring64 xmss_reduced_n32_t151[151];
}
default:
    void;     /* error condition */
};

/* xmss_reduced_array depends on d */
union xmss_reduced_array (xmss_algorithm_type type) {
    case xmssmt-sha2_20/2_256:
        case xmssmt-sha2_20/2_512:
        case xmssmt-sha2_40/2_256:
        case xmssmt-sha2_40/2_512:
        case xmssmt-shake_20/2_256:
        case xmssmt-shake_20/2_512:
        case xmssmt-shake_40/2_256:
        case xmssmt-shake_40/2_512:
            xmss_reduced xmss_red_arr_d2[2];
    case xmssmt-sha2_60/3_256:
        case xmssmt-sha2_60/3_512:
        case xmssmt-shake_60/3_256:
        case xmssmt-shake_60/3_512:
            xmss_reduced xmss_red_arr_d3[3];
    case xmssmt-sha2_20/4_256:
        case xmssmt-sha2_20/4_512:
        case xmssmt-sha2_40/4_256:
        case xmssmt-sha2_40/4_512:
        case xmssmt-shake_20/4_256:
        case xmssmt-shake_20/4_512:
        case xmssmt-shake_40/4_256:
        case xmssmt-shake_40/4_512:
            xmss_reduced xmss_red_arr_d4[4];
    case xmssmt-sha2_60/6_256:
        case xmssmt-sha2_60/6_512:
        case xmssmt-shake_60/6_256:
        case xmssmt-shake_60/6_512:
            xmss_reduced xmss_red_arr_d6[6];
    case xmssmt-sha2_40/8_256:
        case xmssmt-sha2_40/8_512:
        case xmssmt-shake_40/8_256:
        case xmssmt-shake_40/8_512:
            xmss_reduced xmss_red_arr_d8[8];

    

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case xmssmt-sha2_60/12_256:
case xmssmt-sha2_60/12_512:
case xmssmt-shake_60/12_256:
case xmssmt-shake_60/12_512:
    xmss_reduced xmss_red_arr_d12[12];

default:
    void;     /* error condition */
};

/* XMSS^MT signature structure */

struct xmssmt_signature {
    /* WOTS+ key pair index */
    idx_sig_xmssmt idx_sig;
    /* Random string for randomized hashing */
    random_string_xmssmt randomness;
    /* Array of d reduced XMSS signatures */
    xmss_reduced_array;
};

C.3. XMSS^MT Public Keys

XMSS^MT public keys are defined using XDR syntax as follows:

/* Types for bitmask seed */

union seed switch (xmssmt_algorithm_type type) {
    case xmssmt-sha2_20/2_256:
    case xmssmt-sha2_40/4_256:
    case xmssmt-sha2_60/6_256:
    case xmssmt-sha2_20/4_256:
    case xmssmt-sha2_40/8_256:
    case xmssmt-sha2_60/12_256:
    case xmssmt-sha2_40/2_256:
    case xmssmt-sha2_60/3_256:
    case xmssmt-shake_20/2_256:
    case xmssmt-shake_40/4_256:
    case xmssmt-shake_60/6_256:
    case xmssmt-shake_20/4_256:
    case xmssmt-shake_40/8_256:
    case xmssmt-shake_60/12_256:
    case xmssmt-shake_40/2_256:
    case xmssmt-shake_60/3_256:
        bytestring32 seed_n32;
case xmssmt-sha2_20/2_512:
case xmssmt-sha2_20/4_512:
case xmssmt-sha2_20/6_512:
case xmssmt-sha2_20/8_512:
case xmssmt-sha2_20/10_512:
case xmssmt-sha2_20/12_512:
case xmssmt-sha2_20/14_512:
case xmssmt-sha2_20/16_512:
case xmssmt-sha2_20/18_512:
case xmssmt-sha2_20/20_512:
case xmssmt-sha2_20/22_512:
case xmssmt-sha2_20/24_512:
case xmssmt-sha2_20/26_512:
case xmssmt-sha2_20/28_512:
case xmssmt-sha2_20/30_512:
case xmssmt-sha2_20/32_512:
case xmssmt-sha2_20/34_512:
case xmssmt-sha2_20/36_512:
case xmssmt-sha2_20/38_512:
case xmssmt-sha2_20/40_512:
case xmssmt-sha2_20/42_512:
case xmssmt-sha2_20/44_512:
case xmssmt-sha2_20/46_512:
case xmssmt-sha2_20/48_512:
case xmssmt-sha2_20/50_512:
case xmssmt-sha2_20/52_512:
case xmssmt-sha2_20/54_512:
case xmssmt-sha2_20/56_512:
case xmssmt-sha2_20/58_512:
case xmssmt-sha2_20/60_512:
case xmssmt-sha2_20/62_512:
case xmssmt-sha2_20/64_512:
bytestring64 seed_n64;

default:
    void; /* error condition */
};

/* Types for XMSS^MT root node */

union xmssmt_root switch (xmssmt_algorithm_type type) {
    case xmssmt-sha2_20/2_256:
    case xmssmt-sha2_20/4_256:
    case xmssmt-sha2_20/6_256:
    case xmssmt-sha2_20/8_256:
    case xmssmt-sha2_20/10_256:
    case xmssmt-sha2_20/12_256:
    case xmssmt-sha2_20/14_256:
    case xmssmt-sha2_20/16_256:
    case xmssmt-sha2_20/18_256:
    case xmssmt-sha2_20/20_256:
    case xmssmt-sha2_20/22_256:
    case xmssmt-sha2_20/24_256:
    case xmssmt-sha2_20/26_256:
    case xmssmt-sha2_20/28_256:
    case xmssmt-sha2_20/30_256:
    case xmssmt-sha2_20/32_256:
    case xmssmt-sha2_20/34_256:
    case xmssmt-sha2_20/36_256:
    case xmssmt-sha2_20/38_256:
    case xmssmt-sha2_20/40_256:
    case xmssmt-sha2_20/42_256:
    case xmssmt-sha2_20/44_256:
    case xmssmt-sha2_20/46_256:
    case xmssmt-sha2_20/48_256:
    case xmssmt-sha2_20/50_256:
    case xmssmt-sha2_20/52_256:
    case xmssmt-sha2_20/54_256:
    case xmssmt-sha2_20/56_256:
    case xmssmt-sha2_20/58_256:
    case xmssmt-sha2_20/60_256:
    case xmssmt-sha2_20/62_256:
    case xmssmt-sha2_20/64_256:
        bytestring32 root_n32;

case xmssmt-sha2_20/2_512:
    case xmssmt-sha2_20/4_512:
    case xmssmt-sha2_20/6_512:
    case xmssmt-sha2_20/8_512:
    case xmssmt-sha2_20/10_512:
    case xmssmt-sha2_20/12_512:
    case xmssmt-sha2_20/14_512:
    case xmssmt-sha2_20/16_512:
    case xmssmt-sha2_20/18_512:
    case xmssmt-sha2_20/20_512:
    case xmssmt-sha2_20/22_512:
    case xmssmt-sha2_20/24_512:
    case xmssmt-sha2_20/26_512:
    case xmssmt-sha2_20/28_512:
    case xmssmt-sha2_20/30_512:
    case xmssmt-sha2_20/32_512:
    case xmssmt-sha2_20/34_512:
    case xmssmt-sha2_20/36_512:
    case xmssmt-sha2_20/38_512:
    case xmssmt-sha2_20/40_512:
    case xmssmt-sha2_20/42_512:
    case xmssmt-sha2_20/44_512:
    case xmssmt-sha2_20/46_512:
    case xmssmt-sha2_20/48_512:
    case xmssmt-sha2_20/50_512:
    case xmssmt-sha2_20/52_512:
    case xmssmt-sha2_20/54_512:
    case xmssmt-sha2_20/56_512:
    case xmssmt-sha2_20/58_512:
    case xmssmt-sha2_20/60_512:
    case xmssmt-sha2_20/62_512:
    case xmssmt-sha2_20/64_512:
case xmssmt-sha2_60/3_512:
case xmssmt-sha2_60/6_512:
case xmssmt-sha2_60/12_512:
case xmssmt-shake_20/2_512:
case xmssmt-shake_20/4_512:
case xmssmt-shake_40/2_512:
case xmssmt-shake_40/4_512:
case xmssmt-shake_40/8_512:
case xmssmt-shake_60/3_512:
case xmssmt-shake_60/6_512:
case xmssmt-shake_60/12_512:
  bytestring64 root_n64;

  default:
    void;    /* error condition */
  
};

/* XMSS^MT public key structure */

struct xmssmt_public_key {
  xmssmt_root root;  /* Root node */
  seed SEED;  /* Seed for bitmasks */
};

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