### NAME

FingerprintsBitVector

#### **SYNOPSIS**

```
use Fingerprints::FingerprintsBitVector;
use Fingerprints::FingerprintsBitVector qw(:coefficients);
use Fingerprints::FingerprintsBitVector qw(:all);
```

### **DESCRIPTION**

FingerprintsBitVector class provides the following methods:

new, BaroniUrbaniSimilarityCoefficient, BuserSimilarityCoefficient, CosineSimilarityCoefficient, DennisSimilarityCoefficient, DiceSimilarityCoefficient, FoldFingerprintsBitVectorByDensity, FoldFingerprintsBitVectorBySize, ForbesSimilarityCoefficient, FossumSimilarityCoefficient, GetBitsAsBinaryString, GetBitsAsDecimalString, GetBitsAsHexadecimalString, GetBitsAsOctalString, GetBitsAsRawBinaryString, GetDescription, GetFingerprintsBitDensity, GetID, GetSpecifiedSize, GetSupportedSimilarityCoefficients, GetVectorType, HamannSimilarityCoefficient, IsFingerprintsBitVector, IsSubSet, JacardSimilarityCoefficient, Kulczynski1SimilarityCoefficient, MatchingSimilarityCoefficient, Kulczynski2SimilarityCoefficient, MatchingSimilarityCoefficient, McConnaugheySimilarityCoefficient, NewFromBinaryString, NewFromDecimalString, NewFromHexadecimalString, NewFromOctalString, NewFromRawBinaryString, OchiaiSimilarityCoefficient, PearsonSimilarityCoefficient, RogersTanimotoSimilarityCoefficient, RussellRaoSimilarityCoefficient, SetDescription, SetID, SetSpecifiedSize, SetVectorType, SimpsonSimilarityCoefficient, SkoalSneath1SimilarityCoefficient, SkoalSneath2SimilarityCoefficient, TverskySimilarityCoefficient, WeightedTanimotoSimilarityCoefficient, WeightedTverskySimilarityCoefficient, YuleSimilarityCoefficient

The methods available to create fingerprints bit vector from strings and to calculate similarity coefficient between two bit vectors can also be invoked as class functions.

FingerprintsBitVector class is derived from BitVector class which provides the functionality to manipulate bits.

For two fingerprints bit vectors A and B of same size, let:

Hamann: ((Nc + Nd) - (Na - Nc) - (Nb - Nc)) / Nt

Jaccard: Nc / ( ( Na - Nc) + ( Nb - Nc ) + Nc ) = Nc / ( Na + Nb - Nc ) (same as Tanimoto)

Na = Number of bits set to "1" in A Nb = Number of bits set to "1" in B

```
Nc = Number of bits set to "1" in both A and B
Nd = Number of bits set to "0" in both A and B

Nt = Number of bits set to "1" or "0" in A or B (Size of A or B)

Nt = Na + Nb - Nc + Nd

Na - Nc = Number of bits set to "1" in A but not in B
Nb - Nc = Number of bits set to "1" in B but not in A

Then, various similarity coefficients [ Ref. 40 - 42 ] for a pair of bit vectors A and B are defined as follows:

BaroniUrbani: (SQRT(Nc * Nd) + Nc) / (SQRT(Nc * Nd) + Nc + (Na - Nc) + (Nb - Nc)) (same as Buser)

Buser: (SQRT(Nc * Nd) + Nc) / (SQRT(Nc * Nd) + Nc + (Na - Nc) + (Nb - Nc)) (same as BaroniUrbani)

Cosine: Nc / SQRT(Na * Nb) (same as Ochiai)

Dice: (2 * Nc) / (Na + Nb)

Dennis: (Nc * Nd - ((Na - Nc) * (Nb - Nc))) / SQRT(Nt * Na * Nb)

Forbes: (Nt * Nc) / (Na * Nb)

Fossum: (Nt * ((Nc - 1/2) ** 2) / (Na * Nb))
```

```
Kulczynski1: Nc / ((Na - Nc) + (Nb - Nc)) = Nc / (Na + Nb - 2Nc)
           Kulczynski2: ((Nc/2)*(2*Nc+(Na-Nc))+(Nb-Nc)))/((Nc+(Na-Nc))*(Nc+(Nb-Nc))) =
           0.5 * (Nc/Na + Nc/Nb)
           Matching: (Nc + Nd) / Nt
           McConnaughey: ( Nc ** 2 - ( Na - Nc ) * ( Nb - Nc) ) / ( Na * Nb )
           Ochiai: Nc / SQRT (Na * Nb) (same as Cosine)
           Pearson: ((Nc * Nd) - ((Na - Nc) * (Nb - Nc)) / SQRT (Na * Nb * (Na - Nc + Nd) * (Nb - Nc + Nd))
           RogersTanimoto: (Nc + Nd) / ((Na - Nc) + (Nb - Nc) + Nt) = (Nc + Nd) / (Na + Nb - 2Nc + Nt)
           RussellRao: Nc / Nt
           Simpson: Nc / MIN (Na, Nb)
           SkoalSneath1: Nc / (Nc + 2 * (Na - Nc) + 2 * (Nb - Nc)) = Nc / (2 * Na + 2 * Nb - 3 * Nc)
           SkoalSneath2: ( 2 * Nc + 2 * Nd ) / ( Nc + Nd + Nt )
           SkoalSneath3: (Nc + Nd) / ((Na - Nc) + (Nb - Nc)) = (Nc + Nd) / (Na + Nb - 2 * Nc)
           Tanimoto: Nc / ( ( Na - Nc) + ( Nb - Nc ) + Nc ) = Nc / ( Na + Nb - Nc ) (same as Jaccard)
           Tversky: Nc / (alpha * ( Na - Nc ) + ( 1 - alpha) * ( Nb - Nc ) + Nc ) = Nc / (alpha * ( Na - Nb ) + Nb)
           Yule: ( ( Nc * Nd ) - ( ( Na - Nc ) * ( Nb - Nc ) ) ) / ( ( Nc * Nd ) + ( ( Na - Nc ) * ( Nb - Nc ) ) )
           The values of Tanimoto/Jaccard and Tversky coefficients are dependent on only those bit which are set to "1" in
           both A and B. In order to take into account all bit positions, modified versions of Tanimoto [ Ref. 42 ] and Tversky [
           Ref. 43 ] have been developed.
           Let:
               Na' = Number of bits set to "0" in A
               Nb' = Number of bits set to "0" in B
               Nc' = Number of bits set to "0" in both A and B
           Tanimoto': Nc' / ((Na' - Nc') + (Nb' - Nc') + Nc') = Nc' / (Na' + Nb' - Nc')
           Tversky': Nc' / (alpha * (Na' - Nc') + (1 - alpha) * (Nb' - Nc') + Nc') = Nc' / (alpha * (Na' - Nb') + Nb')
           Then:
           WeightedTanimoto = beta * Tanimoto + (1 - beta) * Tanimoto'
           WeightedTversky = beta * Tversky + (1 - beta) * Tversky'
METHODS
           new
                      $NewFPBitVector = new Fingerprints::FingerprintsBitVector($Size);
                  Creates a new FingerprintsBitVector object of size Size and returns newly created FingerprintsBitVector. Bit
                  numbers range from 0 to 1 less than Size.
           BaroniUrbaniSimilarityCoefficient
                      $Value = $FingerprintsBitVector->BaroniUrbaniSimilarityCoefficient(
```

Returns value of BaroniUrbani similarity coefficient between two same size FingerprintsBitVectors.

\$FingerprintsBitVectorA, \$FingerprintBitVectorB);

\$0therFingerprintBitVector);
\$Value = Fingerprints::FingerprintsBitVector::

BaroniUrbaniSimilarityCoefficient(

# Buser Similarity Coefficient

Returns value of Buser similarity coefficient between two same size FingerprintsBitVectors.

### CosineSimilarityCoefficient

Returns value of Cosine similarity coefficient between two same size FingerprintsBitVectors.

### DennisSimilarityCoefficient

Returns value of *Dennis* similarity coefficient between two same size *FingerprintsBitVectors*.

### DiceSimilarityCoefficient

Returns value of Dice similarity coefficient between two same size FingerprintsBitVectors.

### FoldFingerprintsBitVectorByDensity

```
$FingerprintsBitVector->FoldFingerprintsBitVectorByDensity($Density);
```

Folds *FingerprintsBitVector* by recursively reducing its size by half until bit density of set bits is greater than or equal to specified *Density* and returns folded *FingerprintsBitVector*.

# FoldFingerprintsBitVectorBySize

```
$FingerprintsBitVector->FoldFingerprintsBitVectorBySize($Size);
```

Folds *FingerprintsBitVector* by recursively reducing its size by half until size is less than or equal to specified *Size* and returns folded *FingerprintsBitVector*.

### ForbesSimilarityCoefficient

Returns value of Forbes similarity coefficient between two same size FingerprintsBitVectors.

# Fossum Similarity Coefficient

Returns value of Fossum similarity coefficient between two same size FingerprintsBitVectors.

### GetBitsAsBinaryString

```
$BinaryASCIIString = $FingerprintsBitVector->GetBitsAsBinaryString();
```

Returns fingerprints as a binary ASCII string containing 0s and 1s.

```
GetBitsAsHexadecimalString
```

```
$HexadecimalString = $FingerprintsBitVector->GetBitsAsHexadecimalString();
```

Returns fingerprints as a hexadecimal string.

#### GetBitsAsRawBinaryString

```
$RawBinaryString = $FingerprintsBitVector->GetBitsAsRawBinaryString();
```

Returns fingerprints as a raw binary string containing packed bit values for each byte.

### GetDescription

```
$Description = $FingerprintsBitVector->GetDescription();
```

Returns a string containing description of fingerprints bit vector.

### GetFingerprintsBitDensity

```
$BitDensity = $FingerprintsBitVector->GetFingerprintsBitDensity();
```

Returns BitDensity of FingerprintsBitVector corresponding to bits set to 1s.

#### GetI D

```
$ID = $FingerprintsBitVector->GetID();
```

Returns ID of FingerprintsBitVector.

# GetVectorType

```
$VectorType = $FingerprintsBitVector->GetVectorType();
```

Returns VectorType of FingerprintsBitVector.

# GetSpecifiedSize

```
$Size = $FingerprintsBitVector->GetSpecifiedSize();
```

Returns value of specified size for bit vector.

# ${\tt GetSupportedSimilarityCoefficients}$

```
@SimilarityCoefficient =
Fingerprints::FingerprintsBitVector::GetSupportedSimilarityCoefficients();
```

Returns an array containing names of supported similarity coefficients.

## HamannSimilarityCoefficient

Returns value of *Hamann* similarity coefficient between two same size *FingerprintsBitVectors*.

### **IsFingerprintsBitVector**

Returns 1 or 0 based on whether Object is a FingerprintsBitVector object.

# IsSubSet

Returns 1 or 0 based on whether first firngerprints bit vector is a subset of second fingerprints bit vector.

For a bit vector to be a subset of another bit vector, both vectors must be of the same size and the bit positions set in first vector must also be set in the second bit vector.

### JacardSimilarityCoefficient

Returns value of Jacard similarity coefficient between two same size FingerprintsBitVectors.

# Kulczynski1SimilarityCoefficient

Returns value of Kulczynski1 similarity coefficient between two same size FingerprintsBitVectors.

# Kulczynski2SimilarityCoefficient

Returns value of Kulczynski2 similarity coefficient between two same size FingerprintsBitVectors.

### MatchingSimilarityCoefficient

Returns value of *Matching* similarity coefficient between two same size *FingerprintsBitVectors*.

#### McConnaugheySimilarityCoefficient

Returns value of McConnaughey similarity coefficient between two same size FingerprintsBitVectors.

# NewFromBinaryString

Creates a new FingerprintsBitVector using BinaryString and returns new FingerprintsBitVector object.

# NewFromHexadecimalString

Creates a new FingerprintsBitVector using HexdecimalString and returns new FingerprintsBitVector object.

### NewFromRawBinaryString

Creates a new FingerprintsBitVector using RawBinaryString and returns new FingerprintsBitVector object.

# OchiaiSimilarityCoefficient

Returns value of Ochiai similarity coefficient between two same size FingerprintsBitVectors.

# PearsonSimilarityCoefficient

Returns value of *Pearson* similarity coefficient between two same size *FingerprintsBitVectors*.

## RogersTanimotoSimilarityCoefficient

Returns value of RogersTanimoto similarity coefficient between two same size FingerprintsBitVectors.

### RussellRaoSimilarityCoefficient

Returns value of RussellRao similarity coefficient between two same size FingerprintsBitVectors.

## SetSpecifiedSize

```
$FingerprintsBitVector->SetSpecifiedSize($Size);
```

Sets specified size for fingerprints bit vector.

Irrespective of specified size, Perl functions used to handle bit data in BitVector class automatically sets the size to the next nearest power of 2. *SpecifiedSize* is used by FingerprintsBitVector class to process any aribitrary size during similarity coefficient calculations.

# SetDescription

```
$FingerprintsBitVector->SetDescription($Description);
```

Sets *Description* of fingerprints bit vector and returns *FingerprintsBitVector*.

## SetID

```
$FingerprintsBitVector->SetID($ID);
```

Sets ID of fingerprints bit vector and returns FingerprintsBitVector.

#### SetVectorType

```
$FingerprintsBitVector->SetVectorType($VectorType);
```

Sets VectorType of fingerprints bit vector and returns FingerprintsBitVector.

## SimpsonSimilarityCoefficient

Returns value of Simpson similarity coefficient between two same size FingerprintsBitVectors.

### SkoalSneath1SimilarityCoefficient

Returns value of SkoalSneath1 similarity coefficient between two same size FingerprintsBitVectors.

#### SkoalSneath2SimilarityCoefficient

Returns value of SkoalSneath2 similarity coefficient between two same size FingerprintsBitVectors.

# SkoalSneath3SimilarityCoefficient

Returns value of SkoalSneath3 similarity coefficient between two same size FingerprintsBitVectors

# StringifyFingerprintsBitVector

```
$String = $FingerprintsBitVector->StringifyFingerprintsBitVector();
```

Returns a string containing information about FingerprintsBitVector object.

### TanimotoSimilarityCoefficient

Returns value of Tanimoto similarity coefficient between two same size FingerprintsBitVectors.

### TverskySimilarityCoefficient

Returns value of Tversky similarity coefficient between two same size FingerprintsBitVectors.

### WeightedTanimotoSimilarityCoefficient

```
$Value =
    $FingerprintsBitVector->WeightedTanimotoSimilarityCoefficient(
    $0therFingerprintBitVector, $Beta);
$Value =
    Fingerprints::FingerprintsBitVector::
    WeightedTanimotoSimilarityCoefficient(
    $FingerprintsBitVectorA, $FingerprintBitVectorB, $Beta);
```

Returns value of WeightedTanimoto similarity coefficient between two same size FingerprintsBitVectors.

# Weighted Tversky Similarity Coefficient

```
$Value =
   $FingerprintsBitVector->WeightedTverskySimilarityCoefficient(
        $0therFingerprintBitVector, $Alpha, $Beta);
$Value =
   Fingerprints::FingerprintsBitVector::
    WeightedTverskySimilarityCoefficient(
   $FingerprintsBitVectorA, $FingerprintBitVectorB, $Alpha, $Beta);
```

Returns value of WeightedTversky similarity coefficient between two same size FingerprintsBitVectors.

# YuleSimilarityCoefficient

Returns value of Yule similarity coefficient between two same size FingerprintsBitVectors.

### **AUTHOR**

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# SEE ALSO

BitVector.pm, FingerprintsStringUtil.pm, FingerprintsVector.pm, Vector.pm

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