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Title Handle Continuous-Time Quantum Walks with R

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Description Functions and tools for creating, visualizing, and investigating properties of continuous-time quantum walks, including efficient calculation of matrices such as the mixing matrix, average mixing matrix, and spectral decomposition of the Hamiltonian. E. Farhi (1997): <[arXiv:quant-ph/9706062v2](https://arxiv.org/abs/quant-ph/9706062v2)>; C. Godsil (2011) <[arXiv:1103.2578v3](https://arxiv.org/abs/1103.2578v3)>.

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URL <https://github.com/vitormarquesr/qwalkr>,
<https://vitormarquesr.github.io/qwalkr/>

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act_eigfun	<i>Apply a Function to an Operator</i>
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Description

Apply a Function to an Operator

Usage

```
act_eigfun(object, ...)
```

Arguments

object	a representation of the operator.
...	further arguments passed to or from other methods.

Value

The resulting operator from the application of the function.

See Also

[act_eigfun.spectral\(\)](#)

Examples

```
s <- spectral(rbind(c(0.5, 0.3), c(0.3,0.7)))

act_eigfun(s, function(x) x^2) #-> act_eigfun.spectral(...)
```

act_eigfun.spectral *Apply a Function to a Hermitian Matrix*

Description

Apply a function to a Hermitian matrix based on the representation given by class spectral.

Usage

```
## S3 method for class 'spectral'
act_eigfun(object, FUN, ...)
```

Arguments

object	an instance of class spectral.
FUN	the function to be applied to the matrix.
...	further arguments passed on to FUN.

Value

The matrix resulting from the application of FUN.

A Hermitian Matrix admits the spectral decomposition

$$H = \sum_k \lambda_k E_k$$

where λ_k are its eigenvalues and E_k the orthogonal projector onto the λ_k -eigenspace.

If f =FUN is defined on the eigenvalues of H, then act_eigfun performs the following calculation

$$f(H) = \sum_k f(\lambda_k) E_k$$

See Also

[spectral\(\)](#), [act_eigfun\(\)](#)

Examples

```
H <- matrix(c(0,1,1,1,0,1,1,1,0), nrow=3)
decomp <- spectral(H)

# Calculates H^2.
act_eigfun(decomp, FUN = function(x) x^2)

# Calculates sin(H).
act_eigfun(decomp, FUN = function(x) sin(x))

# Calculates H^3.
act_eigfun(decomp, FUN = function(x, y) x^y, 3)
```

avg_matrix

The Average Mixing Matrix of a Quantum Walk

Description

The Average Mixing Matrix of a Quantum Walk

Usage

```
avg_matrix(object, ...)
```

Arguments

object a representation of the quantum walk.
... further arguments passed to or from other methods.

Value

The average mixing matrix.

See Also

[mixing_matrix\(\)](#), [gavg_matrix\(\)](#), [avg_matrix.ctqwalk\(\)](#)

Examples

```
w <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))
avg_matrix(w) #-> avg_matrix.ctqwalk(...)
```

avg_matrix.ctqwalk *The Average Mixing Matrix of a Continuous-Time Quantum Walk*

Description

The Average Mixing Matrix of a Continuous-Time Quantum Walk

Usage

```
## S3 method for class 'ctqwalk'
avg_matrix(object, ...)
```

Arguments

object a representation of the quantum walk.
 ... further arguments passed to or from other methods.

Details

Let $M(t)$ be the mixing matrix of the quantum walk, then the average mixing matrix is defined as

$$\widehat{M} := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T M(t) dt$$

and encodes the long-term average behavior of the walk. Given the Hamiltonian $H = \sum_r \lambda_r E_r$, it is possible to prove that

$$\widehat{M} = \sum_r E_r \circ E_r$$

Value

avg_matrix() returns the average mixing matrix as a square matrix of the same order as the walk.

See Also

[ctqwalk\(\)](#), [avg_matrix\(\)](#)

Examples

```
walk <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))

# Return the average mixing matrix
avg_matrix(walk)
```

 cartesian

Adjacency Matrix of the Cartesian Product

Description

Returns the adjacency matrix of the cartesian product of two graphs given the adjacency matrix of each one, G and H .

Usage

```
cartesian(G, H = NULL)
```

Arguments

G adjacency matrix of the first graph.
 H adjacency matrix of the second graph. If not provided, it takes the same value as G .

Value

Let $A(G)$, $A(H)$ be the adjacency matrices of the graphs G , H such that $|V(G)| = n$ and $|V(H)| = m$, then the adjacency matrix of the cartesian product $G \times H$ is given by

$$A(G \times H) = A(G) \otimes I_{m \times m} + I_{n \times n} \otimes A(H)$$

See Also

[J\(\)](#), [tr\(\)](#), [trdot\(\)](#)

Examples

```
P3 <- matrix(c(0,1,0,1,0,1,0,1,0), nrow=3)
K3 <- matrix(c(0,1,1,1,0,1,1,1,0), nrow=3)

# Return the adjacency matrix of P3 X K3
cartesian(P3, K3)

# Return the adjacency matrix of P3 X P3
cartesian(P3)
```

`ctqwalk`*Create a Continuous-time Quantum Walk*

Description

`ctqwalk()` creates a quantum walk object from a hamiltonian.

Usage

```
ctqwalk(hamiltonian, ...)
```

Arguments

`hamiltonian` a Hermitian Matrix representing the Hamiltonian of the system.
`...` further arguments passed on to [spectral\(\)](#)

Value

A list with the walk related objects, i.e the hamiltonian and its spectral decomposition (See [spectral\(\)](#) for further details)

See Also

[spectral\(\)](#), [unitary_matrix.ctqwalk\(\)](#), [mixing_matrix.ctqwalk\(\)](#), [avg_matrix.ctqwalk\(\)](#), [gavg_matrix.ctqwalk\(\)](#)

Examples

```
# Creates a walk from the adjacency matrix of the graph P3.  
ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))
```

`gavg_matrix`*The Generalized Average Mixing Matrix of a Quantum Walk*

Description

The Generalized Average Mixing Matrix of a Quantum Walk

Usage

```
gavg_matrix(object, ...)
```

Arguments

object a representation of the quantum walk.
 ... further arguments passed to or from other methods.

Value

The generalized average mixing matrix.

See Also

[mixing_matrix\(\)](#), [avg_matrix\(\)](#), [gavg_matrix.ctqwalk\(\)](#)

Examples

```
w <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))
gavg_matrix(w, rnorm(100)) #-> gavg_matrix.ctqwalk(...)
```

gavg_matrix.ctqwalk	<i>The Generalized Average Mixing Matrix of a Continuous-Time Quantum Walk</i>
---------------------	--

Description

The Generalized Average Mixing Matrix of a Continuous-Time Quantum Walk

Usage

```
## S3 method for class 'ctqwalk'
gavg_matrix(object, R, ...)
```

Arguments

object a representation of the quantum walk.
 R samples from the random variable R (For performance, it is recommended at most 10000 samples).
 ... further arguments passed to or from other methods.

Details

Let $M(t)$ be the mixing matrix of the quantum walk and R a random variable with associated probability density function $f_R(t)$. Then the generalized average mixing matrix under R is defined as

$$\widehat{M}_R := \mathbb{E}[M(R)] = \int_{-\infty}^{\infty} M(t) f_R(t) dt$$

Value

gavg_matrix() returns the generalized average mixing matrix as a square matrix of the same order as the walk.

See Also

[ctqwalk\(\)](#), [gavg_matrix\(\)](#)

Examples

```
walk <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))

# Return the average mixing matrix under a Standard Gaussian distribution
gavg_matrix(walk, rnorm(1000))
```

get_eigproj

Extract an Eigen-Projector from an operator

Description

Extract an Eigen-Projector from an operator

Usage

```
get_eigproj(object, ...)
```

Arguments

object a representation of the operator.
... further arguments passed to or from other methods.

Value

A representation of the requested eigen-projector.

See Also

[get_eigspace\(\)](#), [get_eigschur\(\)](#), [get_eigproj.spectral\(\)](#)

Examples

```
s <- spectral(rbind(c(0.5, 0.3), c(0.3,0.7)))

get_eigproj(s, 1) #-> get_eigproj.spectral(...)
```

get_eigproj.spectral *Extract an Eigen-Projector from a Hermitian Matrix*

Description

Get the orthogonal projector associated with an eigenspace based on the representation of a Hermitian Matrix given by class spectral.

Usage

```
## S3 method for class 'spectral'
get_eigproj(object, id, ...)
```

Arguments

object	an instance of class spectral.
id	index for the desired eigenspace according to the ordered (decreasing) spectra.
...	further arguments passed to or from other methods.

Value

The orthogonal projector of the desired eigenspace.

A Hermitian matrix S admits the spectral decomposition $S = \sum_r \lambda_r E_r$ such that E_r is the orthogonal projector onto the λ_r -eigenspace. If V_{id} is the matrix associated to the eigenspace, then

$$E_{id} = V_{id}V_{id}^*$$

See Also

[spectral\(\)](#), [get_eigproj\(\)](#)

Examples

```
# Spectra is {2, -1} with multiplicities one and two respectively.
decomp <- spectral(matrix(c(0,1,1,1,0,1,1,1,0), nrow=3))

# Returns the projector associated to the eigenvalue -1.
get_eigproj(decomp, id=2)

# Returns the projector associated to the eigenvalue 2.
get_eigproj(decomp, id=1)
```

get_eigschur	<i>Extract a Schur Cross-Product from an Operator</i>
--------------	---

Description

Extract a Schur Cross-Product from an Operator

Usage

```
get_eigschur(object, ...)
```

Arguments

object	a representation of the operator.
...	further arguments passed to or from other methods.

Value

A representation of the requested Schur cross-product.

See Also

[get_eigspace\(\)](#), [get_eigproj\(\)](#), [get_eigschur.spectral\(\)](#)

Examples

```
s <- spectral(rbind(c(0.5, 0.3), c(0.3,0.7)))  
get_eigschur(s, 1, 2) #-> get_eigschur.spectral(...)
```

get_eigschur.spectral	<i>Extract a Schur Cross-Product from a Hermitian Matrix</i>
-----------------------	--

Description

Get the Schur product between eigen-projectors based on the representation of a Hermitian Matrix given by class `spectral`.

Usage

```
## S3 method for class 'spectral'  
get_eigschur(object, id1, id2 = NULL, ...)
```

Arguments

object	an instance of class spectral.
id1	index for the first eigenspace according to the ordered (decreasing) spectra.
id2	index for the second eigenspace according to the ordered (decreasing) spectra. If not provided, it takes the same value as id1.
...	further arguments passed to or from other methods.

Value

The Schur product of the corresponding eigenprojectors, $E_{id_1} \circ E_{id_2}$.

See Also

[spectral\(\)](#), [get_eigschur\(\)](#)

Examples

```
# Spectra is {2, -1} with multiplicities one and two respectively.
decomp <- spectral(matrix(c(0,1,1,1,0,1,1,1,0), nrow=3))

# Returns the Schur product between the 2-projector and -1-projector.
get_eigschur(decomp, id1=2, id2=1)

# Returns the Schur square of the 2-projector.
get_eigschur(decomp, id1=1, id2=1)

# Also returns the Schur square of the 2-projector
get_eigschur(decomp, id1=1)
```

get_eigspace

Extract an Eigenspace from an Operator

Description

Extract an Eigenspace from an Operator

Usage

```
get_eigspace(object, ...)
```

Arguments

object	a representation of the operator.
...	further arguments passed to or from other methods.

Value

A representation of the requested eigenspace.

See Also

[get_eigproj\(\)](#), [get_eigschur\(\)](#), [get_eigspace.spectral\(\)](#)

Examples

```
s <- spectral(rbind(c(0.5, 0.3), c(0.3,0.7)))
get_eigspace(s, 1) #-> get_eigspace.spectral(...)
```

get_eigspace.spectral *Extract an Eigenspace from a Hermitian Matrix*

Description

Get the eigenbasis associated with an eigenvalue based on the representation of a Hermitian Matrix given by class spectral.

Usage

```
## S3 method for class 'spectral'
get_eigspace(object, id, ...)
```

Arguments

object	an instance of class spectral.
id	index for the desired eigenspace according to the ordered (decreasing) spectra.
...	further arguments passed to or from other methods.

Value

A matrix whose columns form the orthonormal eigenbasis.

If $s \leftarrow \text{spectral}(A)$ and $V \leftarrow s\$eigvectors$, then the extracted eigenspace V_{id} is some submatrix $V[, _]$.

See Also

[spectral\(\)](#), [get_eigspace\(\)](#)

Examples

```
# Spectra is {2, -1} with multiplicities one and two respectively.
decomp <- spectral(matrix(c(0,1,1,1,0,1,1,1,0), nrow=3))

# Returns the two orthonormal eigenvectors corresponding to the eigenvalue -1.
get_eigspace(decomp, id=2)

# Returns the eigenvector corresponding to the eigenvalue 2.
get_eigspace(decomp, id=1)
```

J

The All-Ones Matrix

Description

Returns the all-ones matrix of order n .

Usage

`J(n)`

Arguments

`n` the order of the matrix.

Value

A square matrix of order n in which every entry is equal to 1. The all-ones matrix is given by $J_{n \times n} = \mathbf{1}_n \mathbf{1}_n^T$.

See Also

[tr\(\)](#), [trdot\(\)](#), [cartesian\(\)](#)

Examples

```
# Return the all-ones matrix of order 5.
J(5)
```

mixing_matrix *The Mixing Matrix of a Quantum Walk*

Description

The Mixing Matrix of a Quantum Walk

Usage

```
mixing_matrix(object, ...)
```

Arguments

object a representation of the quantum walk.
... further arguments passed to or from other methods.

Value

The mixing matrix of the quantum walk.

See Also

[unitary_matrix\(\)](#), [avg_matrix\(\)](#), [gavg_matrix\(\)](#), [mixing_matrix.ctqwalk\(\)](#)

Examples

```
w <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))  
mixing_matrix(w, t = 2*pi) #-> mixing_matrix.ctqwalk(...)
```

mixing_matrix.ctqwalk *The Mixing Matrix of a Continuous-Time Quantum Walk*

Description

The Mixing Matrix of a Continuous-Time Quantum Walk

Usage

```
## S3 method for class 'ctqwalk'  
mixing_matrix(object, t, ...)
```

Arguments

object	an instance of class ctqwalk.
t	it will be returned the mixing matrix at time t.
...	further arguments passed to or from other methods.

Details

Let $U(t)$ be the time evolution operator of the quantum walk at time t , then the mixing matrix is given by

$$M(t) = U(t) \circ \overline{U(t)}$$

$M(t)$ is a doubly stochastic real symmetric matrix, which encodes the probability density of the quantum system at time t .

More precisely, the $(M(t))_{ab}$ entry gives us the probability of measuring the standard basis state $|b\rangle$ at time t , given that the quantum walk started at $|a\rangle$.

Value

mixing_matrix() returns the mixing matrix of the CTQW evaluated at time t.

See Also

[ctqwalk\(\)](#), [mixing_matrix\(\)](#)

Examples

```
walk <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))

# Returns the mixing matrix at time t = 2*pi, M(2pi)
mixing_matrix(walk, t = 2*pi)
```

```
print.ctqwalk
```

Print the ctqwalk output

Description

Print the ctqwalk output

Usage

```
## S3 method for class 'ctqwalk'
print(x, ...)
```


Arguments

`x` an object of the class `ctqwalk`.
`...` further arguments passed to or from other methods.

Value

Called mainly for its side effects. However, also returns `x` invisibly.

spectral *Spectral Decomposition of a Hermitian Matrix*

Description

`spectral()` is a wrapper around `base::eigen()` designed for Hermitian matrices, which can handle repeated eigenvalues.

Usage

```
spectral(S, multiplicity = TRUE, tol = .Machine$double.eps^0.5, ...)
```

Arguments

`S` a Hermitian matrix. *Obs:* The matrix is always assumed to be Hermitian, and only its lower triangle (diagonal included) is used.

`multiplicity` if TRUE (default), tries to infer eigenvalue multiplicity. If set to FALSE, each eigenvalue is considered unique with multiplicity one.

`tol` two eigenvalues `x`, `y` are considered equal if $\text{abs}(x-y) < \text{tol}$. Defaults to $\text{tol} = \text{.Machine\$double.eps}^0.5$.

`...` further arguments passed on to `base::eigen()`

Value

The spectral decomposition of `S` is returned as a list with components

`eigvals` vector containing the unique eigenvalues of `S` in *decreasing* order.

`multiplicity` multiplicities of the eigenvalues in `eigvals`.

`eigvectors` a $\text{nrow}(S) \times \text{nrow}(S)$ unitary matrix whose columns are eigenvectors ordered according to `eigvals`. Note that there may be more eigenvectors than eigenvalues if `multiplicity=TRUE`, however eigenvectors of the same eigenspace are next to each other.

The Spectral Theorem ensures the eigenvalues of `S` are real and that the vector space admits an orthonormal basis consisting of eigenvectors of `S`. Thus, if `s <- spectral(S)`, and `V <- s$eigvectors`; `lam <- s$eigvals`, then

$$S = V\Lambda V^*$$

where $\Lambda = \text{diag}(\text{rep}(\text{lam}, \text{times}=\text{s\$multiplicity}))$

See Also

[base::eigen\(\)](#), [get_eigspace.spectral\(\)](#), [get_eigproj.spectral\(\)](#), [get_eigschur.spectral\(\)](#),
[act_eigfun.spectral\(\)](#)

Examples

```
spectral(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))

# Use "tol" to set the tolerance for numerical equality
spectral(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3), tol=10e-5)

# Use "multiplicity=FALSE" to force each eigenvalue to be considered unique
spectral(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3), multiplicity = FALSE)
```

tr

The Trace of a Matrix

Description

Computes the trace of a matrix A.

Usage

```
tr(A)
```

Arguments

A a square matrix.

Value

If A has order n , then $tr(A) = \sum_{i=1}^n a_{ii}$.

See Also

[J\(\)](#), [trdot\(\)](#), [cartesian\(\)](#)

Examples

```
A <- rbind(1:5, 2:6, 3:7)

# Calculate the trace of A
tr(A)
```

`trdot`*The Trace Inner Product of Matrices*

Description

Computes the trace inner product of two matrices A and B.

Usage

```
trdot(A, B)
```

Arguments

A, B square matrices.

Value

The trace inner product on $Mat_{n \times n}(\mathbb{C})$ is defined as

$$\langle A, B \rangle := tr(A^* B)$$

See Also

[J\(\)](#), [tr\(\)](#), [cartesian\(\)](#)

Examples

```
A <- rbind(1:5, 2:6, 3:7)
B <- rbind(7:11, 8:12, 9:13)

# Compute the trace inner product of A and B
trdot(A, B)
```

`unitary_matrix`*The Unitary Time Evolution Operator of a Quantum Walk*

Description

The Unitary Time Evolution Operator of a Quantum Walk

Usage

```
unitary_matrix(object, ...)
```

Arguments

object a representation of the quantum walk.
 ... further arguments passed to or from other methods.

Value

The unitary time evolution operator.

See Also

[mixing_matrix\(\)](#), [unitary_matrix.ctqwalk\(\)](#)

Examples

```
w <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))
unitary_matrix(w, t = 2*pi) #-> unitary_matrix.ctqwalk(...)
```

unitary_matrix.ctqwalk

The Unitary Time Evolution Operator of a Continuous-Time Quantum Walk

Description

The Unitary Time Evolution Operator of a Continuous-Time Quantum Walk

Usage

```
## S3 method for class 'ctqwalk'
unitary_matrix(object, t, ...)
```

Arguments

object an instance of class ctqwalk.
 t it will be returned the evolution operator at time t.
 ... further arguments passed to or from other methods.

Details

If $|\psi(t)\rangle$ is the quantum state of the system at time t , and H the Hamiltonian operator, then the evolution is governed by the Schrodinger equation

$$\frac{\partial}{\partial t}|\psi(t)\rangle = iH|\psi(t)\rangle$$

and if H is time-independent its solution is given by

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = e^{iHt}|\psi(0)\rangle$$

The evolution operator is the result of the complex matrix exponential and it can be calculated as

$$U(t) = e^{iHt} = \sum_r e^{it\lambda_r} E_r$$

in which $H = \sum_r \lambda_r E_r$.

Value

`unitary_matrix()` returns the unitary time evolution operator of the CTQW evaluated at time `t`.

See Also

[ctqwalk\(\)](#), [unitary_matrix\(\)](#), [act_eigfun\(\)](#)

Examples

```
walk <- ctqwalk(matrix(c(0,1,0,1,0,1,0,1,0), nrow=3))  
  
# Returns the operator at time t = 2*pi, U(2pi)  
unitary_matrix(walk, t = 2*pi)
```

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