Dynamic, Dynamic > MatrixX< double > + Rows + Cols + areEqualEigenvaluesAs() + isEqualEigenvectorAs() + hasEqualSetsOfEigenvectorsAs() + operator()() + operator()() + calculateMinor() + Eigen() + Eigen() + isPositiveSemiDefinite() + pairWiseReduced() + print() + removeColumn() + removeColumns() + removeRow() + removeRows() + FromColumnMajorVector() + FromFile() + FromFile() + FromRowMajorVector() GQCP::Matrix < double > + Rows + Cols + areEqualEigenvaluesAs() + isEqualEigenvectorAs() + hasEqualSetsOfEigenvectorsAs() + operator()() + operator()() + calculateMinor() + Eigen() + Eigen() + isPositiveSemiDefinite() + pairWiseReduced() + print() + removeColumn() + removeColumns() + removeRow() + removeRows() + FromColumnMajorVector() + FromFile() + FromFile() + FromRowMajorVector() GQCP::SquareMatrix < double > + SquareMatrix() + SquareMatrix() + SquareMatrix() + SquareMatrix() ${\sf GQCP::} Base Orbital Optimizer$ + SquareMatrix() + dimension() # is_converged + isSelfAdjoint() # convergence threshold + isHermitian() # maximum_number_of_iterations + isAntiHermitian() # number_of_iterations + isSymmetric() #gradient + BaseOrbitalOptimizer() + noPivotLUDecompose() + ~BaseOrbitalOptimizer() + pairWiseStrictReduced() + calculatePermanentCombinatorial() + calculateNewRotationMatrix() + calculatePermanentRyser() + checkForConvergence() + prepareConvergenceChecking() + FromStrictTriangle() + numberOfIterations() + Identity() + PartitionMatrix() + optimize() + PartitionMatrix() + Random() + RandomSymmetric() + RandomUnitary() + SymmetricFromUpperTriangle() + SymmetricFromUpperTriangle WithoutDiagonal() + Zero() #hessian GQCP::NewtonOrbitalOptimizer # hessian_modifier + NewtonOrbitalOptimizer() + ~NewtonOrbitalOptimizer() + calculateGradientMatrix() + calculateHessianTensor() + calculateNewFullOrbitalGenerators() + prepareOrbitalDerivatives Calculation() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + calculateGradientVector() + calculateHessianMatrix() + calculateNewFreeOrbitalGenerators() + directionFromIndefiniteHessian() + newtonStepIsWellDefined() GQCP::ERNewtonLocalizer + ERNewtonLocalizer() + calculateGradientMatrix() + calculateHessianTensor() + calculateNewFullOrbitalGenerators() + prepareOrbitalDerivatives

Calculation()

+ calculateGradientMatrixElement()
+ calculateHessianTensorElement()

Eigen::Matrix < double,