GQCP::BaseOrbitalOptimizer # is converged # convergence threshold # maximum_number_of_iterations # number_of_iterations + BaseOrbitalOptimizer() + ~BaseOrbitalOptimizer() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + numberOfIterations() + optimize() GQCP::NewtonOrbitalOptimizer GQCP::JacobiOrbitalOptimizer # hessian modifier # dim # gradient # optimal jacobi with # hessian scalar + NewtonOrbitalOptimizer() + JacobiOrbitalOptimizer() + ~NewtonOrbitalOptimizer() + ~JacobiOrbitalOptimizer() + calculateGradientMatrix() + calculatelacobiCoefficients() + calculateHessianTensor() + calculateOptimalRotation + calculateNewFullOrbitalGenerators() + prepareOrbitalDerivatives + calculateScalarFunctionChange() Calculation() + preparelacobiSpecificConvergence + calculateNewRotationMatrix() + checkForConvergence() Checking() + calculateNewRotationMatrix() + prepareConvergenceChecking() + checkForConvergence() + calculateGradientVector() + prepareConvergenceChecking() + calculateHessianMatrix() + calculateOptimalJacobiParameters() + calculateNewFreeOrbitalGenerators() + directionFromIndefiniteHessian() + comparer() + newtonStepIsWellDefined() GOCP::QCMethodNewtonOrbital Optimizer GQCP::AP1roGJacobiOrbital GQCP::ERNewtonLocalizer Optimizer # D GQCP::ERJacobiLocalizer + ~QCMethodNewtonOrbitalOptimizer() + AP1roGJacobiOrbitalOptimizer() + ERNewtonLocalizer() + calculateJacobiCoefficients() + calculate1DM() + calculateGradientMatrix() + AP1roGlacobiOrbitalOptimizer() + calculateOptimalRotation + calculate2DM() + calculateJacobiCoefficients() + calculateHessianTensor() + prepareDMCalculation() Angle() + calculateOptimalRotation + calculateNewFullOrbitalGenerators() + calculateGradientMatrix() + calculateScalarFunctionChange() Angle() + prepareOrbitalDerivatives + prepareJacobiSpecificConvergence + calculateHessianTensor() Calculation() + calculateScalarFunctionChange() + prepareOrbitalDerivatives + prepareJacobiSpecificConvergence + calculateGradientMatrixElement() + JacobiOrbitalOptimizer() Calculation() Checking() + calculateHessianTensorElement() + oneDM() + electronicEnergy() + twoDM() + NewtonOrbitalOptimizer() GQCP::AP1roGLagrangianNewton OrbitalOptimizer + AP1roGLagrangianNewtonOrbital Optimizer() + AP1roGLagrangianNewtonOrbital Optimizer() + prepareDMCalculation() + calculate1DM() + calculate2DM() + calculateNewFullOrbitalGenerators() + electronicEnergy() + geminalCoefficients() + multipliers()