## GQCP::BaseOrbitalOptimizer

- # is\_converged
- # convergence threshold
- # maximum\_number\_of\_iterations
- # number of iterations
- + BaseOrbitalOptimizer()
- + ~BaseOrbitalOptimizer()
- + calculateNewRotationMatrix()
- + checkForConvergence()
- + prepareConvergenceChecking()
- + numberOfIterations()
- + optimize()



## GQCP::JacobiOrbitalOptimizer

- # dim
- # optimal\_jacobi\_with
- scalar
- + JacobiOrbitalOptimizer()
- + ~JacobiOrbitalOptimizer()
- + calculateJacobiCoefficients()
- + calculateOptimalRotation
- Angle()
  - + calculateScalarFunctionChange()
  - + prepareJacobiSpecificConvergence
  - Checking()
  - + calculateNewRotationMatrix()
  - + checkForConvergence()
  - + prepareConvergenceChecking()
  - + calculateOptimalJacobiParameters()
  - + comparer()



## GQCP::AP1roGJacobiOrbital Optimizer

- + AP1roGJacobiOrbitalOptimizer()
- + AP1roGJacobiOrbitalOptimizer()
- + calculateJacobiCoefficients()
- + calculateOptimalRotation Angle()
- + calculateScalarFunctionChange()
- + prepareJacobiSpecificConvergence Checking()
- + electronicEnergy()