Optimization of Model Parameters and Experimental Designs for a Global Marine Biogeochemical Model

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Outline

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Motivation

Simplified schematic of the global carbon cycle from the IPCC Report 2013.
The PO₄-DOP Model

- models phosphate (PO₄) and dissolved organic phosphorus (DOP)
- computes also the mass of produced phytoplankton
- coupled with an ocean circulation model
- annual periodic state
- computational expensive
- resolution: 3h, 15 depth layers, 2.8125° at each layer
- seven inaccurately known model parameters

Exemplary model output.
Measurement Data

- DOP: around 400 measurements from three different cruises
- PO$_4$: over 4 million measurements from World Ocean Database 2013

Distribution of PO$_4$ measurements

- Near the surface (upper 25 m, 1° grid)
- Per 50 m depth, per year, per day
Mean and Standard Deviation

Interpolated mean of PO$_4$ concentrations.

Interpolated standard deviation of PO$_4$ concentrations.

near the surface, averaged in time
Correlation

- highly correlated measurements
- correlation depending on positions (not only on distance)
- dense matrix would need over 64TB, sparse matrices used
- size influenceable by minimal number of measurements
- if not positive definite, approximate with positive definite matrix
- Cholesky decomposition with permutation
Parameter Optimization

- generalized least squares cost function $\phi(p) = (F(p) - d)^T C^{-1} (F(p) - d)$
- box constraints
- SQP algorithm as local optimization algorithm
- OQNLP algorithm as global optimization algorithm
- cost function scaled
- derivatives calculated with finite differences with speedup
Uncertainty Quantification (model parameters)

- uncertainty in measurements results in uncertainty in optimal parameters
- inverse Fisher information matrix as estimation of covariance matrix of parameter estimator
- computationally more expensive approaches not applicable
Uncertainty Quantification (model output)

- uncertainty in optimal parameters results in uncertainty in corresponding model output
- asymptotic variance of the model output estimator as measure of uncertainty in optimal model output
Optimal Experimental Design

- optimization of additional measurements
- different types possible
- exemplary optimization done with genetic algorithms

average model confidence increase by one additional measurement
Workflow

1. Plan measurements
2. Carry out measurements
3. Estimate model parameters
4. Estimate uncertainties
5. Accurate enough?
   - Yes
   - No

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Parameter Estimation in a BGC Model
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