MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Quantifying Uncertainty: Nonlinear Input-Output Systems

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Bosch Innovation Workshop

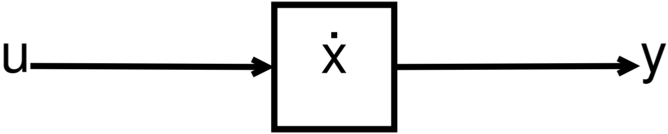
Uncertainty Quantification (UQ)

UQ: an attempt of a definition:

- Computation of statistical quantities
- for models based on differential equations
- that include uncertain components
- of which distributions can be modeled.

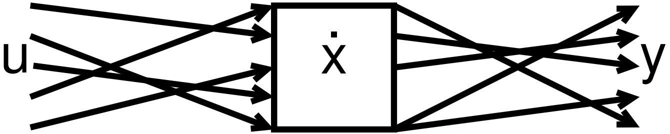
- **Practically**:
  Inverse problems, Bayesian inference, forward propagation
- **Mathematically**:
  Parameter Hessians, parameter identification, Many-query setting

Input-Output System



- **Input** u (excitation, boundary term)
- Grey box **model** $\dot{x}$ (ODE, semi-discrete PDE)
- **Output** y (sensors, QoI)

Uncertain Systems



- Input uncertainty (i.e.: uniformly random scaling)
- Model uncertainty (i.e.: uncertain vector field)
- Output uncertainty (i.e: additive Gaussian noise)

What's an Uncertainty?

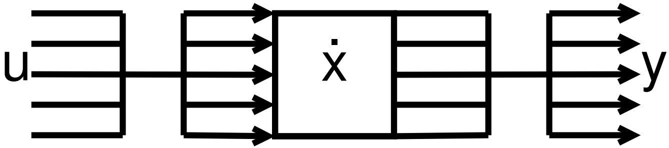
Uncertainty:

- Possible sources: measurement, modeling, material, ...
- Defined in terms of a distribution,
  - often assumed Gaussian via mean and covariance,
- usually determined from experiments.

Parametric perspective:

- Uncertainties are basically parameters,
- whereas the distribution defines the relevant range
- and importance of parameter intervals.

Parametric System



- Input-to-State parametrization
- State parametrization
- State-to-Output-parametrization

Mathematical System

Input-output system:

$$\dot{x}(t) = f(x(t), u(t), \theta)$$
$$y(t) = g(x(t), u(t), \theta)$$

- Vector field f
- Output functional g
- Input function $u(t)$
- State trajectory $x(t)$
- Output function $y(t)$
- Parameters θ

Parametric Model Reduction

Reduced order model:

$$\dot{x}_r(t) = f_r(x_r(t), u(t), \theta)$$
$$y_r(t) = g_r(x_r(t), u(t), \theta)$$

- Reduced vector field f_r
- Reduced output functional g_r
- Reduced state trajectory $x_r(t)$
- Approximate output function $y_r(t)$
- $\dim(x(t)) \ll \dim(x_r(t))$
- $\|y(\theta) - y_r(\theta)\| \ll 1$

System Covariance

Covariance:
An indicator of dependence between two variables.

Covariance properties:

- Linear operator,
- symmetric,
- positive (semi-)definite.

System Covariance:
An indicator of dependence between two state components (x_i, x_j).

Covariance matrix:
A matrix of all pairwise dependencies between state components.

Controllability and Observability

- **Controllability**[1]: Ability to drive states by inputs.
- **Observability**: Ability to infer states from outputs.

Model reduction via balanced truncation:

- The least controllable
- and least observable

states are least important to input-output coherence.

Balanced truncation features:

- Based on associated system Gramian matrices,
- sort balanced states by Hankel singular values,
- stability-preserving reduced order model,
- global $\mathcal{H}_\infty / L_2$ error bound.

[1] Often actually **Reachability** is meant as for linear systems they are equivalent.

Empirical Gramians

- **Empirical**: Data-driven computation.
- **Gramian**: A special type of covariance matrix.

Empirical Gramian matrix types:

- Empirical Controllability Gramian
- Empirical Observability Gramian
- Empirical Cross Gramian (combines controllability and observability)

Computation outline:

1. Determine operating region,
2. perturb input, states / parameters (uncertainties),
3. simulate (output) trajectory,
4. assemble covariance (Gramian) matrix,
5. accumulate by averaging.

Back to UQ

How does this help with UQ?

1. Assume uncertainties are parameters.
2. Assume parameters are (constant) states.

$$\begin{pmatrix} \dot{x}(t) \\ \dot{\theta}(t) \end{pmatrix} = \begin{pmatrix} f(x(t), u(t), \theta(t)) \\ 0 \end{pmatrix}$$
$$y(t) = g(x(t), u(t), \theta(t))$$

State and parameter reduced order system:

$$\dot{x}_r(t) = f_r(x_r(t), u(t), \theta_r)$$
$$y_r(t) = g_r(x_r(t), u(t), \theta_r)$$

- Reduced vector field f_r
- Reduced output functional g_r
- Reduced state trajectory $x_r(t)$
- Approximate output function $y_r(t)$
- $\dim(x_r) \ll \dim(x)$
- $\dim(\theta_r) \ll \dim(\theta)$
- $\|y(\theta) - y_r(\theta_r)\| \ll 1$

Gramian-Based Combined Reduction

Treating parameters as inputs (**controllability**-based):

- Empirical Sensitivity Gramian

Treating parameters as states (**observability**-based):

- Empirical Identifiability Gramian
- Empirical Cross-Identifiability Gramian

Parameter identification:

- Eigenvalue decomposition (EVD)
- Singular value decomposition (SVD)
- Principal component analysis (PCA)

Empirical Gramians:

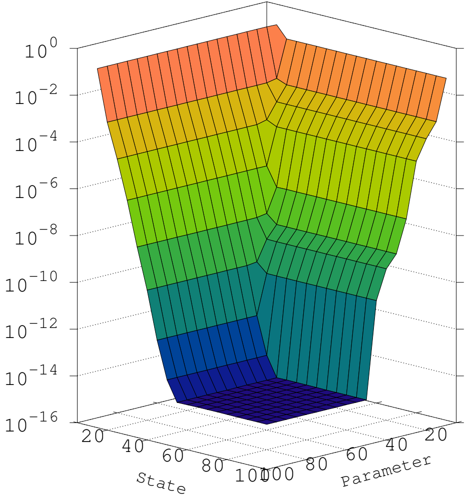
- Empirical Controllability Gramian
- Empirical Observability Gramian
- Empirical Linear Cross Gramian
- Empirical Cross Gramian
- Empirical Sensitivity Gramian (controllability-based state + parameter)
- Empirical Identifiability Gramian (observability-based state + parameter)
- Empirical Joint Gramian (cross-based state + observability-based parameter)

Features:

- Interfaces for: Solver, inner product kernels & distributed memory
- Non-Symmetric option for all cross Gramians
- Compatible with OCTAVE and MATLAB
- Vectorized and parallelizable
- Open-source licensed

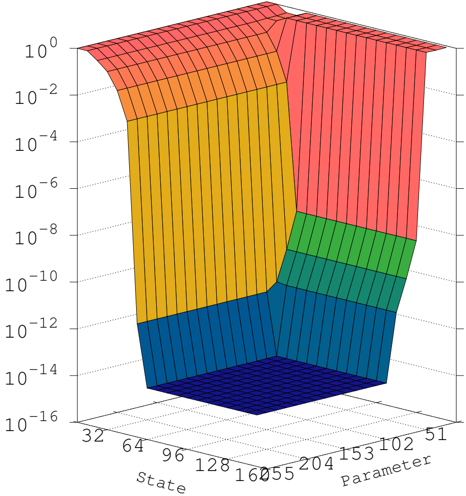
More info: `http://gramian.de`

Weakly nonlinear, linear parametrized system:



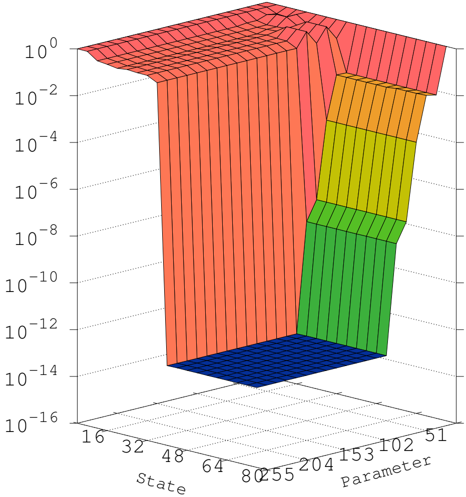
Relative model reduction error for varying state and parameter dimensions.

Weakly nonlinear, second order, nonlinear parametrized system:



Relative model reduction error for varying state and parameter dimensions.

Highly nonlinear, nonlinear parametrized system:



Relative model reduction error for varying state and parameter dimensions.

Summary

In a nutshell:

- Treat uncertainties as parameters,
- treat parameters as states,
- perturb states,
- sort by observability (and controllability).

Ingredients:

- Spatially-discrete model
- Operating region
- Full order model solver

Further Works I: POD and RBM

Proper Orthogonal Decomposition (POD)[2] for UQ

- Treat uncertainties as parameters.
- Extract relevant state-space information from a time-series
- for multiple time-series at relevant sampling points.

Reduced Basis Method (RBM)[3] for UQ

- Treat uncertainties as parameters.
- Build a reduced basis for a high order finite element basis.
- Typically: use a greedy method to select sampling points

[2] P. Benner and J. Schneider. **Uncertainty Quantification for Maxwell's Equations Using Stochastic Collocation and Model Order Reduction**. International Journal for Uncertainty Quantification, 5(3): 195–208, 2015.

[3] P. Benner and M.W. Hess. **Reduced Basis Modeling for Uncertainty Quantification of Electromagnetic Problems in Stochastically Varying Domains**. In: Scientific Computing in Electrical Engineering, Springer, Mathematics in Industry vol. 23: 215–222, 2016.

Further Works II: Krylov Subspaces

Krylov Subspaces[4] [5] for UQ

- Treat uncertainties as parameters.
- Build a basis by repeated application of differential operator.
- Extract relevant moments valid over parameter domain.
- Generalization of the moment-matching model reduction method.

[4] Y. Yue, S. Li, L. Feng, A. Seidel-Morgenstern and P. Benner. **Efficient Model Reduction of SMB Chromatography by Krylov-subspace Method with Application in Uncertainty Quantification**. 24th Symposium on Computer-Aided Process Engineering, vol. 33: 925–930, 2014.

[5] Y. Yue, L. Feng, P. Meuris, W. Schoenmaker and P. Benner. **Application of Krylov-type Parametric Model Order Reduction in Efficient Uncertainty Quantification of Electro-thermal Circuit Models**. Progress in Electromagnetics Research Symposium Proceedings: 379–384, 2015.

Next

Discussion points:

- What are the goals of using UQ?
- What are relevant models and model classes?
- What is the dimensionality of the models?

References:

[1] A.C. Antoulas. **Approximation of Large-Scale Dynamical Systems**, volume 6 of Advances in Design and Control. SIAM, 2005. ISBN 9780898715293

[2] P. Benner, S. Gugercin, and K. Willcox. **A survey of model reduction methods for parametric systems**. SIAM Review, 57(4):483–531, 2015.

[3] C. Himpe. **Combined State and Parameter Reduction for Nonlinear Systems with an Application in Neuroscience**. PhD thesis, Westfälische Wilhelms-Universität Münster, 2017. Sierke Verlag Göttingen, ISBN 9783868448818

[4] U. Baur, P. Benner, B. Haasdonk, C. Himpe, I. Martini, and M. Ohlberger. **Comparison of methods for parametric model order reduction of instationary problems**. In P. Benner, A. Cohen, M. Ohlberger, and K. Willcox, editors, Model Reduction and Approximation: Theory and Algorithms. To Appear, 2017.

- These slides: `http://himpe.science/talks/himpe17-bosch.pdf`