Exploiting Sparsity in Bayesian Inverse Problems of Parametric Operator Equations

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SAM

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Outline

Inverse Problem

Physical Model

$$G(u) \to \delta$$

- u parameter vector / parameter function
- G the forward map modelling the physical process
- δ result / observations

Forward Problem

Find the output δ for given parameters u

$\to$ **well-posed**

Inverse Problem

Find the parameters u from (noisy) observations δ

$\to$ **ill-posed**

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

- u parameter vector / parameter function
- G the forward map modelling the physical process
- $\mathcal{O}$ bounded, linear observation operator
- $\mathcal{G}$ uncertainty-to-observation map, $\mathcal{G} = \mathcal{O} \circ G$
- δ noisy observations
- η observational noise

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

Deterministic optimization problem

$$\min_u \frac{1}{2}\|\delta - \mathcal{G}(u)\|^2 + R(u)$$

- $\|\delta - \mathcal{G}(u)\|$ potential / data misfit
- R regularization term

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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Deterministic optimization problem

$$\min_u \frac{1}{2} \|\delta - \mathcal{G}(u)\|^2 + R(u)$$

- **Large-scale, deterministic optimization problem**
- **No quantification of the uncertainty in the unknown $\mathbf{u}$**
- **Proper choice of the regularization term $\mathbf{R}$**

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

Bayesian inverse problem

$$\delta = \mathcal{G}(u) + \eta$$

- u, η, δ random variables / fields
- Goal of computation: moments of system quantities under the posterior w.r. to noisy data δ

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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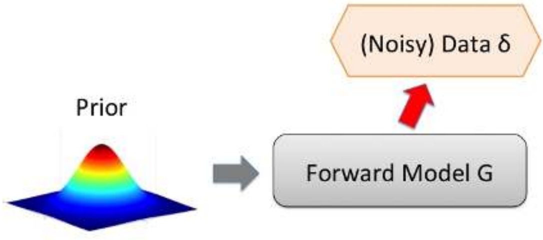
Bayesian inverse problem



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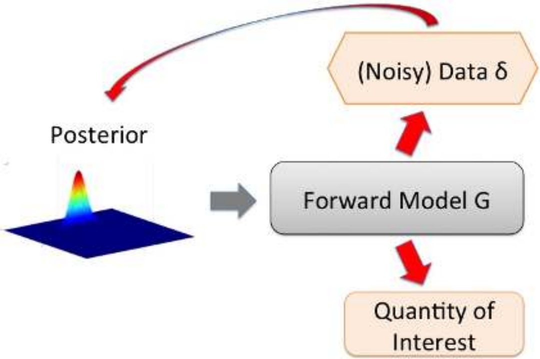

Inverse Problem

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Bayesian inverse problem

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- **Quantification of uncertainty in $\mathbf{u}$ and system quantities**
- **Well-posedness of the inverse problem**
- **Incorporation of prior knowledge on the uncertain data $\mathbf{u}$**
- **Need of efficient approximations of the posterior**

Bayesian Inverse Problems (Stuart 2010)

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

Goal: Efficient estimation of system quantities from noisy observations

- Infinite-dimensional parameter space
- Fast convergence by exploiting sparsity of the underlying forward problem
- Suitable for application to a broad class of forward problems

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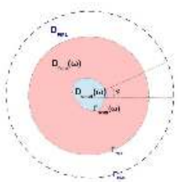
UQ in Nano Optics



Bayesian Inverse Problems (Stuart 2010)

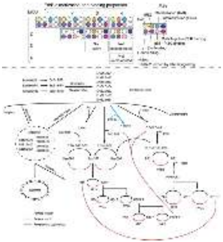
Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

Goal: Efficient estimation of system quantities from noisy observations

UQ in Biochemical Networks

- Infinite-dimensional parameter space
- Fast convergence by exploiting sparsity of the underlying forward problem
- Suitable for application to a broad class of forward problems



Source: Chen et al.

Bayesian Inverse Problems (Stuart 2010)

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

- X separable Banach space
- $G : X \mapsto \mathcal{X}$ the forward map

Abstract Operator Equation

$$\text{Given } u \in X, \text{ find } q \in \mathcal{X} : \quad A(u;q) = F(u) \quad \text{in} \quad \mathcal{Y}'$$

with $A(u;\cdot) \in \mathcal{L}(\mathcal{X}, \mathcal{Y}')$, $F : X \mapsto \mathcal{Y}'$, $\mathcal{X}$, $\mathcal{Y}$ reflexive Banach spaces,
$\mathfrak{a}(v,w) :=_{\mathcal{Y}} \langle w, Av \rangle_{\mathcal{Y}'}$ $\forall v \in \mathcal{X}, w \in \mathcal{Y}$ corresponding bilinear form

- $\mathcal{O} : \mathcal{X} \mapsto \mathbb{R}^K$ bounded, linear observation operator
- $\mathcal{G} : X \mapsto \mathbb{R}^K$ uncertainty-to-observation map, $\mathcal{G} = \mathcal{O} \circ G$
- $\eta \in \mathbb{R}^K$ the observational noise ($\eta \sim \mathcal{N}(0, \Gamma)$)

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Least squares potential $\Phi : X \times \mathbb{R}^K \to \mathbb{R}$

$$\Phi(u; \delta) := \frac{1}{2}\Big((\delta - \mathcal{G}(u))^\top \Gamma^{-1} (\delta - \mathcal{G}(u))\Big)$$

Reformulation of the forward problem with unknown stochastic input data as an infinite dimensional, parametric deterministic problem

Bayesian Inverse Problems (Stuart 2010)

Parametric representation of the unknown u

$$u = u(\boldsymbol{y}) := \langle u \rangle + \sum_{j \in \mathbb{J}} y_j \psi_j \in X$$

- $\boldsymbol{y} = (y_j)_{j \in \mathbb{J}}$ iid sequence of real-valued random variables $y_j \sim \mathcal{U}[-1, 1]$
- $\langle u \rangle, \psi_j \in X$
- $\mathbb{J}$ finite or countably infinite index set

Prior measure on the uncertain input data

$$\mu_0(d\boldsymbol{y}) := \bigotimes_{j \in \mathbb{J}} \frac{1}{2} \lambda_1(dy_j) \, .$$

- $(U, \mathcal{B}) = \left([-1, 1]^{\mathbb{J}}, \ \bigotimes_{j \in \mathbb{J}} \mathcal{B}^1[-1, 1] \right)$ measurable space

Bayesian Inverse Problem

Theorem (ChS and Stuart 2011)

Assume that $\mathcal{G}(u)\Big|_{u=\langle u\rangle+\sum_{j\in\mathbb{J}} y_j\psi_j}$ is bounded and continuous.

Then $\mu^\delta(d\boldsymbol{y})$, the distribution of $\boldsymbol{y}\in U$ given δ, is absolutely continuous with respect to $\mu_0(d\boldsymbol{y})$, and

$$\frac{d\mu^\delta}{d\mu_0}(\boldsymbol{y}) = \frac{1}{Z}\Theta(\boldsymbol{y})$$

with the parametric Bayesian posterior Θ given by

$$\Theta(\boldsymbol{y}) = \exp\big(-\Phi(u;\delta)\big)\Big|_{u=\langle u\rangle+\sum_{j\in\mathbb{J}} y_j\psi_j},$$

and the normalization constant

$$Z = \int_U \Theta(\boldsymbol{y})\mu_0(d\boldsymbol{y})\ .$$

Bayesian Inverse Problem

Expectation of a *Quantity of Interest* $\phi : X \to S$

$$\mathbb{E}^{\mu^\delta}[\phi(u)] = Z^{-1} \int_U \exp\big(-\Phi(u;\delta)\big)\phi(u)\Big|_{u=\langle u\rangle+\sum_{j\in\mathbb{J}} y_j\psi_j} \mu_0(d\boldsymbol{y}) =: Z'/Z$$

with $Z = \mathbb{E}^{\mu^\delta}[1] = \int_U \exp(-\frac{1}{2}\left((\delta - \mathcal{G}(u))^\top \Gamma^{-1}(\delta - \mathcal{G}(u))\right))\mu_0(d\boldsymbol{y})$.

- Reformulation of the forward problem with unknown stochastic input data as an infinite dimensional, parametric deterministic problem
- Parametric, deterministic representation of the derivative of the posterior measure with respect to the prior μ_0
- Approximation of Z' and Z to compute the expectation of QoI under the posterior given data δ

Efficient algorithm to approximate the conditional expectations given the data with dimension-independent rates of convergence

Bayesian Inverse Problem

Expectation of a *Quantity of Interest* $\phi : X \to S$

$$\mathbb{E}^{\mu^\delta}[\phi(u)] = Z^{-1} \int_U \exp\big(-\Phi(u;\delta)\big)\phi(u)\Big|_{u=\langle u\rangle+\sum_{j\in\mathbb{J}} y_j\psi_j} \mu_0(d\boldsymbol{y}) =: Z'/Z$$

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Exploiting sparsity in the parametric operator equation

- Parameters belonging to a specified sparsity class
- Analytic regularity of the parametric, deterministic Bayesian posterior
- Parametric, deterministic Bayesian posterior belongs to the same sparsity class

$\to$ **Sparsity of Legendre pce + dimension-independent convergence rates for Smolyak integration algorithms**

$(\boldsymbol{b}, p, \epsilon)$-Analyticity

$(\boldsymbol{b}, p, \epsilon) : 1$ (well-posedness)

For each $\boldsymbol{y} \in U$, there exists a unique realization $u(\boldsymbol{y}) \in X$ and a unique solution $q(\boldsymbol{y}) \in \mathcal{X}$ of the forward problem. This solution satisfies the a-priori estimate

$$\forall \boldsymbol{y} \in U : \quad \|q(\boldsymbol{y})\|_{\mathcal{X}} \leq C_0 \,.$$

$(\boldsymbol{b}, p, \epsilon) : 2$ (analyticity)

There exist $0 < p < 1$ and $\boldsymbol{b} = (b_j)_{j \in \mathbb{J}} \in \ell^p(\mathbb{J})$ such that for $\epsilon > 0$, there exist $C_\epsilon > 0$ and $\rho = (\rho_j)_{j \in \mathbb{J}}$ of poly-radii $\rho_j > 1$ such that

$$\sum_{j \in \mathbb{J}} (\rho_j - 1) b_j \leq \epsilon \,,$$

and $U \ni \boldsymbol{y} \mapsto q(\boldsymbol{y}) \in \mathcal{X}$ admits an analytic continuation to the open polyellipse $\mathcal{E}_\rho := \prod_{j \in \mathbb{J}} \mathcal{E}_{\rho_j} \subset \mathbb{C}^{\mathbb{J}}$ with

$$\forall \boldsymbol{z} \in \mathcal{E}_\rho : \quad \|q(\boldsymbol{z})\|_{\mathcal{X}} \leq C_\epsilon \,.$$

$(\boldsymbol{b}, p, \epsilon)$-Analyticity of Parametric Operator Families

$$u \in X : A(u;q) = F(u) \quad q \in \mathcal{X}$$

Assumption A1

For $\epsilon > 0$ and some $0 < p < 1$, there exists a positive sequence $\boldsymbol{b} = (b_j)_{j\geq 1} \in \ell^p(\mathbb{N})$, such that for any sequence $\rho := (\rho_j)_{j\geq 1}$ $\rho := (\rho_j)_{j\geq 1}$ with $\rho_j > 1,\ \sum_{j\in\mathbb{J}}(\rho_j - 1)b_j \leq \epsilon$, $\mathfrak{a}$ and F are holomorphic in $\mathcal{E}_\rho$.

Assumption A2

The holomorphic extensions satisfy the uniform continuity conditions

$$\sup_{w\in\mathcal{Y}\setminus\{0\}} \frac{|f(z;w)|}{\|w\|_\mathcal{Y}} \leq M, \qquad \sup_{v\in\mathcal{X}\setminus\{0\}, w\in\mathcal{Y}\setminus\{0\}} \frac{|\mathfrak{a}(z;v,w)|}{\|v\|_\mathcal{X}\|w\|_\mathcal{Y}} \leq R,$$

with $M < \infty, f$ corresponding linear form of F.

Assumption A3

There hold the uniform inf-sup conditions:

$$\inf_{v\in\mathcal{X}\setminus\{0\}} \sup_{w\in\mathcal{Y}\setminus\{0\}} \frac{|\mathfrak{a}(z;v,w)|}{\|v\|_\mathcal{X}\|w\|_\mathcal{Y}} \geq r \quad \text{und} \quad \inf_{w\in\mathcal{Y}\setminus\{0\}} \sup_{v\in\mathcal{X}\setminus\{0\}} \frac{|\mathfrak{a}(z;v,w)|}{\|v\|_\mathcal{X}\|w\|_\mathcal{Y}} \geq r$$

with $0 < r \leq R < \infty$.

$(\boldsymbol{b}, p, \epsilon)$-Analyticity of Parametric Operator Families

$$u \in X : A(u;q) = F(u) \quad q \in \mathcal{X}$$

Assumption A1 $\mathfrak{a}$ and F holomorphic in $\mathcal{E}_\rho$
Assumption A2

$$\sup_{w \in \mathcal{Y} \setminus \{0\}} \frac{|f(z;w)|}{\|w\|_{\mathcal{Y}}} \leq M, \qquad \sup_{v \in \mathcal{X} \setminus \{0\}, w \in \mathcal{Y} \setminus \{0\}} \frac{|\mathfrak{a}(z;v,w)|}{\|v\|_{\mathcal{X}} \|w\|_{\mathcal{Y}}} \leq R$$

Assumption A3

$$\inf_{v \in \mathcal{X} \setminus \{0\}} \sup_{w \in \mathcal{Y} \setminus \{0\}} \frac{|\mathfrak{a}(z;v,w)|}{\|v\|_{\mathcal{X}} \|w\|_{\mathcal{Y}}} \geq r \quad \text{und} \quad \inf_{w \in \mathcal{Y} \setminus \{0\}} \sup_{v \in \mathcal{X} \setminus \{0\}} \frac{|\mathfrak{a}(z;v,w)|}{\|v\|_{\mathcal{X}} \|w\|_{\mathcal{Y}}} \geq r$$

Theorem (Cohen, Chkifa, ChS 2013)

Unter Assumptions **A1 - A3**, $\mathcal{A}(u;q) = A(u;q) - F(u)$ satisfies the $(\boldsymbol{b}, p, \epsilon)$-holomorphy assumptions.

Sparsity of the Forward Solution

Theorem (Chkifa, Cohen, DeVore and ChS)

Assume that the parametric forward solution map $q(\boldsymbol{y})$ admits a $(\boldsymbol{b}, p, \epsilon)$-analytic extension to the poly-ellipse $\mathcal{E}_\rho \subset \mathbb{C}^{\mathbb{J}}$.

- The Legendre series converges unconditionally,

$$q(\boldsymbol{y}) = \sum_{\nu \in \mathcal{F}} q_\nu^P P_\nu(\boldsymbol{y}) \quad \text{in } L^\infty(U, \mu_0; \mathcal{X})$$

  with Legendre polynomials $P_k(1) = 1,\ \|P_k\|_{L^\infty(-1,1)} = 1\ , \quad k = 0, 1, ...$

- There exists a p-summable, monotone envelope $\boldsymbol{q} = \{\boldsymbol{q}_\nu\}_{\nu \in \mathcal{F}}$, i.e. $\boldsymbol{q}_\nu := \sup_{\mu \geq \nu} \|q_\nu^P\|_{\mathcal{X}}$ with $C(p, \boldsymbol{q}) := \|\boldsymbol{q}\|_{\ell^p(\mathcal{F})} < \infty$.
  and monotone $\Lambda_N^P \subset \mathcal{F}$ corresponding to the N largest terms of $\boldsymbol{q}$ with

$$\sup_{\boldsymbol{y} \in U} \left\| q(\boldsymbol{y}) - \sum_{\nu \in \Lambda_N^P} q_\nu^P P_\nu(\boldsymbol{y}) \right\|_{\mathcal{X}} \leq C(p, \boldsymbol{q}) N^{-(1/p-1)} \ .$$

Sparsity of the Posterior

Theorem (ClS and ChS 2013)

Assume that the forward solution map $U \ni \boldsymbol{y} \mapsto q(\boldsymbol{y})$ is $(\boldsymbol{b}, p, \epsilon)$–analytic for some $0 < p < 1$.
Then the Bayesian posterior $\Theta(\boldsymbol{y})$ is, as a function of the parameter $\boldsymbol{y}$, likewise $(\boldsymbol{b}, p, \epsilon)$–analytic, with the same p and the same ϵ.

Sketch of proof

- Establish holomorphy of the complex extension Θ on the poly-ellipse $\mathcal{E}_\rho \subset \mathbb{C}^{\mathbb{J}}$
- Derive bounds on the modulus of the posterior

$$\sup_{\boldsymbol{z}\in\mathcal{E}_\rho} |\Theta(\boldsymbol{z})| \leq \exp\left(\sup_{\boldsymbol{z}\in\mathcal{E}_\rho} \frac{1}{2} \mathrm{Im}\left(\mathcal{G}(u(\boldsymbol{z}))\right)^\top \Gamma^{-1} \mathrm{Im}\left(\mathcal{G}(u(\boldsymbol{z}))\right) \right)$$

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N-term Approximation Results

$$\sup_{\boldsymbol{y} \in U} \left\| \Theta(\boldsymbol{y}) - \sum_{\nu \in \Lambda_N^P} \Theta_\nu^P P_\nu(\boldsymbol{y}) \right\|_{\mathcal{X}} \leq N^{-s} \|\boldsymbol{\theta}^P\|_{\ell_m^p(\mathcal{F})}, \quad s := \frac{1}{p} - 1 \ .$$

Adaptive Smolyak quadrature algorithm with convergence rates depending only on the summability of the parametric operator

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Examples

- Parametric initial value ODEs (Hansen & ChS; Vietnam J. Math. 2013)
- Affine-parametric, linear operator equations (ClS & ChS; 2013)
- Semilinear elliptic PDEs (Hansen & ChS; Math. Nachr. 2013)
- Elliptic multiscale problems (Hoang & ChS; Analysis and Applications 2012)
- Nonaffine holomorphic-parametric, nonlinear problems (Cohen, Chkifa & ChS; 2013)

Univariate Quadrature

Univariate quadrature operators of the form

$$Q^k(\mathtt{g}) = \sum_{i=0}^{n_k} w_i^k \cdot \mathtt{g}(z_i^k)$$

with $\mathtt{g} : [-1, 1] \mapsto \mathbb{R}$.

- $(Q^k)_{k\geq 0}$ sequence of univariate quadrature formulas
- $(z_j^k)_{j=0}^{n_k} \subset [-1, 1]$ with $z_j^k \in [-1, 1]\,, \forall j, k$ and $z_0^k = 0\,, \forall k$ quadrature points
- $w_j^k\,, 0 \leq j \leq n_k,\ \forall k \in \mathbb{N}_0$ quadrature weights

Assumption

(i) $(I - Q^k)(g_k) = 0\,, \quad \forall g_k \in \mathbb{P}_k = \mathrm{span}\{y^j : j \in \mathbb{N}_0, j \leq k\}$
with $I(g_k) = \int_{[-1,1]} g_k(y)\lambda_1(dy)$

(ii) $w_j^k > 0\,, \qquad 0 \leq j \leq n_k,\ \forall k \in \mathbb{N}_0$.

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- $w_j^k\,, 0 \leq j \leq n_k,\ \forall k \in \mathbb{N}_0$ quadrature weights

Univariate quadrature difference operator

$$\Delta_j = Q^j - Q^{j-1}, \qquad j \geq 0$$

with $Q^{-1} = 0$ and $z_0^0 = 0, w_0^0 = 1$.

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- $w_j^k\,, 0 \leq j \leq n_k,\ \forall k \in \mathbb{N}_0$ quadrature weights

Univariate quadrature operator rewritten as telescoping sum

$$Q^k = \sum_{j=0}^{k} \Delta_j$$

with $\mathcal{Z}^k = \{z_j^k : 0 \leq j \leq n_k\} \subset [-1,1]$ set of points corresponding to Q^k.

Sparse Quadrature Operator

Tensorized multivariate operators

$$\mathcal{Q}_\nu = \bigotimes_{j\geq 1} Q^{\nu_j}\,, \qquad \Delta_\nu = \bigotimes_{j\geq 1} \Delta_{\nu_j}$$

with associated set of multivariate points $\mathcal{Z}^\nu = \times_{j\geq 1}\mathcal{Z}^{\nu_j} \in U$.

- If $\nu = 0_\mathcal{F}$, then $\Delta_\nu g = Q^\nu g = g(z_{0_\mathcal{F}}) = g(0_\mathcal{F})$
- If $0_\mathcal{F} \neq \nu \in \mathcal{F}$, with $\hat{\nu} = (\nu_j)_{j\neq i}$

$$Q^\nu g = Q^{\nu_i}(t \mapsto \bigotimes_{j\geq 1} Q^{\hat{\nu}_j} g_t)\,, \qquad i \in \mathbb{I}_\nu$$

and

$$\Delta_\nu g = \Delta_{\nu_i}(t \mapsto \bigotimes_{j\geq 1} \Delta_{\hat{\nu}_j} g_t)\,, \qquad i \in \mathbb{I}_\nu\,,$$

for $g \in \mathcal{Z}$, g_t is the function defined on $\mathcal{Z}^\mathbb{N}$ by
$g_t(\hat{y}) = g(y), y = (\ldots, y_{i-1}, t, y_{i+1}, \ldots)\,, i > 1$ and $y = (t, y_2, \ldots)\,, i = 1$

Sparse Quadrature Operator

For any finite monotone set $\Lambda \subset \mathcal{F}$, the quadrature operator is defined by

$$\mathcal{Q}_\Lambda = \sum_{\nu \in \Lambda} \Delta_\nu = \sum_{\nu \in \Lambda} \bigotimes_{j \geq 1} \Delta_{\nu_j}$$

with associated collocation grid

$$\mathcal{Z}_\Lambda = \cup_{\nu \in \Lambda} \mathcal{Z}^\nu \, .$$

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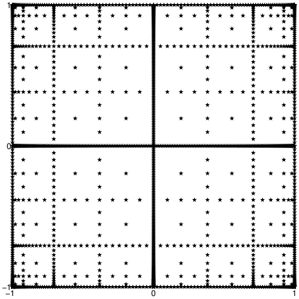

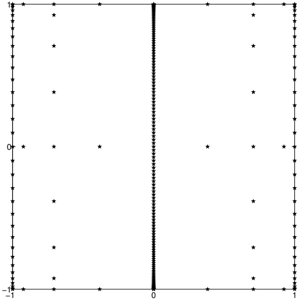

Convergence Rates for Adaptive Smolyak Integration

Theorem

Assume that the forward solution map $U \ni \boldsymbol{y} \mapsto q(\boldsymbol{y})$ is $(\boldsymbol{b}, p, \epsilon)$–analytic for some $0 < p < 1$.

Then there exists a sequence $(\Lambda_N)_{N \geq 1}$ of monotone index sets $\Lambda_N \subset \mathcal{F}$ such that $\#\Lambda_N \leq N$ and

$$|I[\Theta] - \mathcal{Q}_{\Lambda_N}[\Theta]| \leq C^1 N^{-s}\,,$$

with $s = 1/p - 1$, $I[\Theta] = \int_U \Theta(y)\mu_0(d\boldsymbol{y})$ and,

$$\|I[\Psi] - \mathcal{Q}_{\Lambda_N}[\Psi]\|_{\mathcal{X}} \leq C^2 N^{-s}\,, \qquad s = \frac{1}{p} - 1\,.$$

with $I[\Psi] = \int_U \Psi(y)\mu_0(d\boldsymbol{y})$, $C^1, C^2 > 0$ independent of N.

Remark: SAME index sets Λ_N for BOTH, Z' and Z.

ClS and ChS Sparsity in Bayesian Inversion of Parametric Operator Equations, 2013.

Convergence Rates for Adaptive Smolyak Integration

Sketch of proof

- Relating the quadrature error with the Legendre coefficients

$$|I(\Theta) - \mathcal{Q}_\Lambda(\Theta)| \leq 2 \cdot \sum_{\nu \notin \Lambda} \gamma_\nu |\theta_\nu^P|$$

  and

$$\|I(\Psi) - \mathcal{Q}_\Lambda(\Psi)\|_\mathcal{X} \leq 2 \cdot \sum_{\nu \notin \Lambda} \gamma_\nu \|\psi_\nu^P\|_\mathcal{X}$$

  for any monotone set $\Lambda \subset \mathcal{F}$, where $\gamma_\nu := \prod_{j \in \mathbb{J}} (1 + \nu_j)^2$.

- $(\gamma_\nu |\theta_\nu^P|)_{\nu \in \mathcal{F}} \in l_m^p(\mathcal{F})$ and $(\gamma_\nu \|\psi_\nu^P\|_\mathcal{X})_{\nu \in \mathcal{F}} \in l_m^p(\mathcal{F})$.

$\Rightarrow \exists$ sequence $(\Lambda_N)_{N \geq 1}$ of monotone sets $\Lambda_N \subset \mathcal{F}$, $\#\Lambda_N \leq N$, such that the Smolyak quadrature converges with order $1/p - 1$.

Adaptive Construction of the Monotone Index Set

Successive identification of the N largest contributions

$$|\Delta_\nu(\Theta)| = \Big|\bigotimes_{j\geq 1} \Delta_{\nu_j}(\Theta)\Big|\,, \quad \nu \in \mathcal{F}$$

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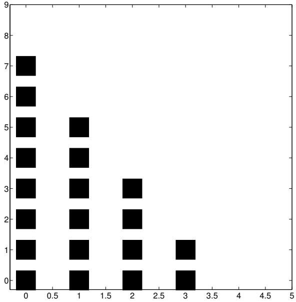
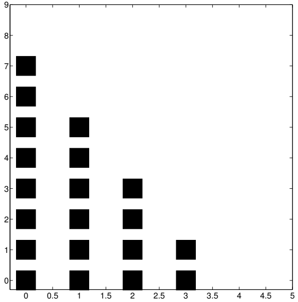
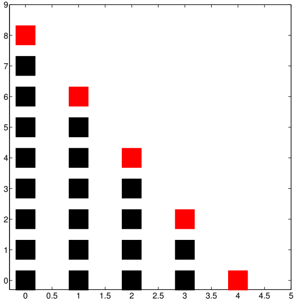


Adaptive Construction of the Monotone Index Set

Successive identification of the N largest contributions

$$|\Delta_\nu(\Theta)| = \Big|\bigotimes_{j\geq 1} \Delta_{\nu_j}(\Theta)\Big|, \quad \nu \in \mathcal{F}$$





Adaptive Construction of the Monotone Index Set

Successive identification of the N largest contributions

$$|\Delta_\nu(\Theta)| = \Big|\bigotimes_{j\geq 1} \Delta_{\nu_j}(\Theta)\Big|, \quad \nu \in \mathcal{F}$$

$\rightarrow$ A. Chkifa, A. Cohen and ChS. High-dimensional adaptive sparse polynomial interpolation and applications to parametric PDEs, 2012.

Reduced set of neighbors

$$\mathcal{N}(\Lambda) := \{\nu \notin \Lambda : \nu - e_j \in \Lambda, \forall j \in \mathbb{I}_\nu \text{ and } \nu_j = 0\,, \forall j > j(\Lambda) + 1\}$$

with $j(\Lambda) = \max\{j : \nu_j > 0 \text{ for some } \nu \in \Lambda\}$, $\mathbb{I}_\nu = \{j \in \mathbb{N} : \nu_j \neq 0\} \subset \mathbb{N}$.

Adaptive Construction of the Monotone Index Set

function ASG
  Set $\Lambda_1 = \{0\}\,, k = 1$ and compute $\Delta_0(\Theta)$.
  Determine the reduced set of neighbors $\mathcal{N}(\Lambda_1)$.
  Compute $\Delta_\nu(\Theta)\,, \forall \nu \in \mathcal{N}(\Lambda_1)$.
  while $\sum_{\nu \in \mathcal{N}(\Lambda_k)} |\Delta_\nu(\Theta)| > tol$ **do**
    Select $\nu \in \mathcal{N}(\Lambda_k)$ with largest $|\Delta_\nu|$ and set $\Lambda_{k+1} = \Lambda_k \cup \{\nu\}$.
    Determine the reduced set of neighbors $\mathcal{N}(\Lambda_{k+1})$.
    Compute $\Delta_\nu(\Theta)\,, \forall \nu \in \mathcal{N}(\Lambda_{k+1})$.
    Set $k = k + 1$.
  end while
end function

T. Gerstner and M. Griebel. Dimension-adaptive tensor-product quadrature, *Computing*, 2003

Numerical Experiments

Model parametric parabolic problem

$$
\begin{aligned}
\partial_t q(t,x) - \mathrm{div}(u(x)\nabla q(t,x)) &= 100 \cdot tx \qquad && (t,x) \in T \times D\,,\\
q(0,x) &= 0 && x \in D\,,\\
q(t,0) = q(t,1) &= 0 && t \in T
\end{aligned}
$$

with

$$u(x,y) = \langle u \rangle + \sum_{j=1}^{64} y_j \psi_j\,, \text{where } \langle u \rangle = 1 \text{ and } \psi_j = \alpha_j \chi_{D_j}$$

where $D_j = [(j-1)\frac{1}{64}, j\frac{1}{64}]$, $y = (y_j)_{j=1,\dots,64}$ and $\alpha_j = \frac{0.9}{j^\zeta}$, $\zeta = 2, 3, 4$.

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
- Uniform mesh with meshwidth $h_T = h_D = 2^{-11}$
- LAPACK's DPTSV routine

Numerical Experiments

Find the unknown data u for given (noisy) data δ,

$$\delta = \mathcal{G}(u) + \eta \,,$$

Expectation of interest Z'/Z

$$\begin{aligned} Z' &= \int_U \exp\big(-\Phi(u;\delta)\big)\phi(u)\Big|_{u=\langle u\rangle + \sum_{j=1}^{64} y_j\psi_j} \mu_0(dy) \\ Z &= \int_U \exp\big(-\Phi(u;\delta)\big)\Big|_{u=\langle u\rangle + \sum_{j=1}^{64} y_j\psi_j} \mu_0(dy) \end{aligned}$$

- Observation operator $\mathcal{O}$ consists of system responses at K observation points in $T \times D$ at $t_i = \frac{i}{2^{N_{K,T}}}, i = 1, \dots, 2^{N_{K,T}} - 1$, $x_j = \frac{j}{2^{N_{K,D}}}, k = 1, \dots, 2^{N_{K,D}} - 1$, $o_k(\cdot,\cdot) = \delta(\cdot - t_k)\delta(\cdot - x_k)$ with $K = 3,\ N_{K,D} = 2,\ N_{K,T} = 1$
- $\mathcal{G} : X \to \mathbb{R}^K$, with $\phi(u) = G(u)$
- $\eta = (\eta_j)_{j=1,\dots,K}$ iid with $\eta_j \sim \mathcal{N}(0,1)$

Numerical Experiments

Quadrature points

- Clenshaw-Curtis (CC)

$$
\begin{aligned}
z_j^k &= -cos\left(\frac{\pi j}{n_k - 1}\right), j = 0, \ldots, n_k - 1, \text{if } n_k > 1 \text{ and} \\
z_0^k &= 0\,, \text{if } n_k = 1
\end{aligned}
$$

with $n_0 = 1$ and $n_k = 2^k + 1,$ for $k \geq 1$

- $\Re$-Leja sequence (RL)

Numerical Experiments

Quadrature points

- Clenshaw-Curtis (CC)
- $\mathfrak{R}$-Leja sequence (RL)
  projection on $[-1, 1]$ of a Leja sequence for the complex unit disk initiated at i

$$
\begin{aligned}
z_0^k &= 0\,, z_1^k = 1\,, z_2^k = -1\,, \text{if } j = 0, 1, 2 \text{ and} \\
z_j^k &= \mathfrak{R}(\hat{z}), \text{ with } \hat{z} = \underset{|z| \le 1}{\operatorname{argmax}} \prod_{l=1}^{j-1} |z - z_l^k|\,, j = 3, \ldots, n_k, \text{if } j \text{ odd}\,, \\
z_j^k &= -z_{j-1}^k\,, j = 3, \ldots, n_k, \text{if } j \text{ even}\,,
\end{aligned}
$$

with $n_k = 2 \cdot k + 1,$ for $k \ge 0$

J.-P. Calvi and M. Phung Van. On the Lebesgue constant of Leja sequences for the unit disk and its applications to multivariate interpolation *Journal of Approximation Theory*, 2011.

J.-P. Calvi and M. Phung Van. Lagrange interpolation at real projections of Leja sequences for the unit disk *Proceedings of the American Mathematical Society*, 2012.

A. Chkifa. On the Lebesgue constant of Leja sequences for the unit disk *Journal of Approximation Theory*, 2013.

Normalization Constant Z

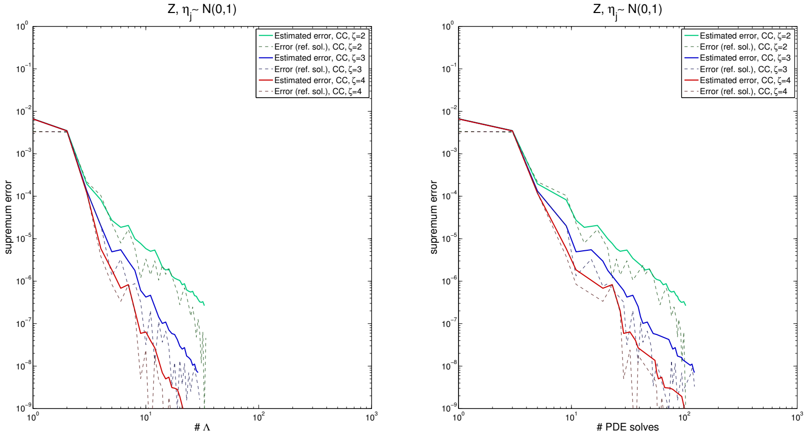


Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the normalization constant Z w.r. to the cardinality of the index set Λ_N (l.) and w.r. to the PDE solves needed (r.) based on the sequence CC with $K = 3$, $\eta \sim \mathcal{N}(0,1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.

Normalization Constant Z

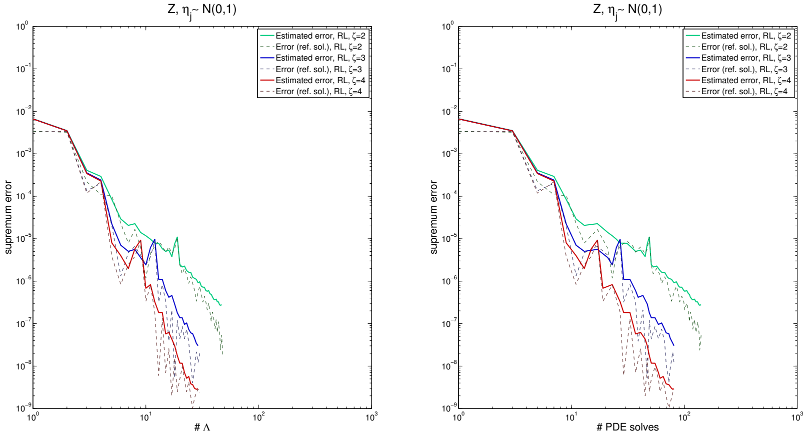
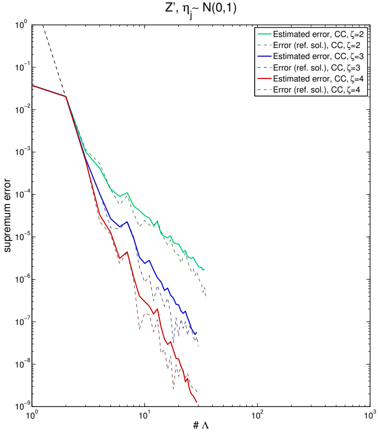
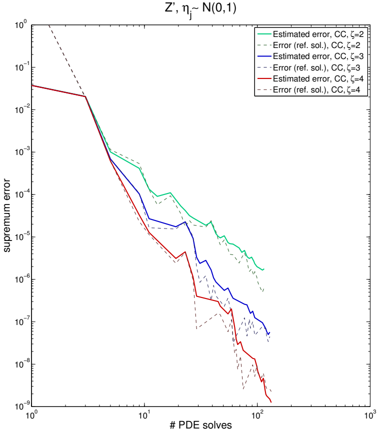


Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the normalization constant Z w.r. to the cardinality of the index set Λ_N (l.) and w.r. to the PDE solves needed (r.) based on the sequence RL with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.

Quantity Z'





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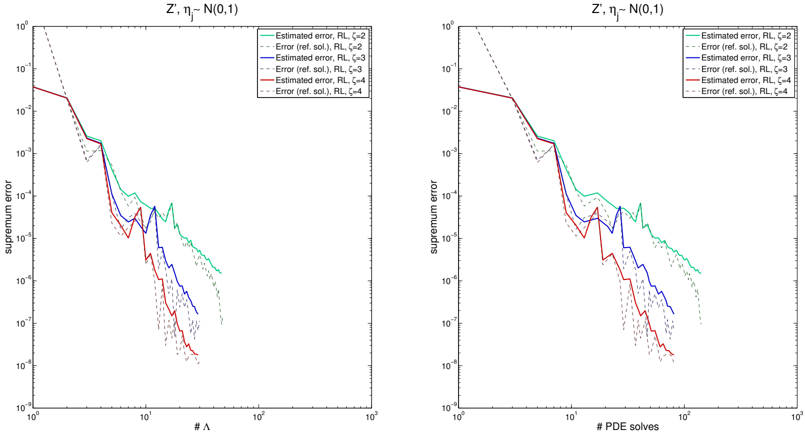

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q(t,0) = q(t,1) &= 0 && t \in T
\end{aligned}
$$

with

$$u(x,y) = \langle u \rangle + \sum_{j=1}^{128} y_j \psi_j\,, \text{where } \langle u \rangle = 1 \text{ and } \psi_j = \alpha_j \chi_{D_j}$$

where $D_j = [(j-1)\frac{1}{128}, j\frac{1}{128}]$, $y = (y_j)_{j=1,\dots,128}$ and $\alpha_j = \frac{0.6}{j^\zeta}\,, \zeta = 2, 3, 4$.

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
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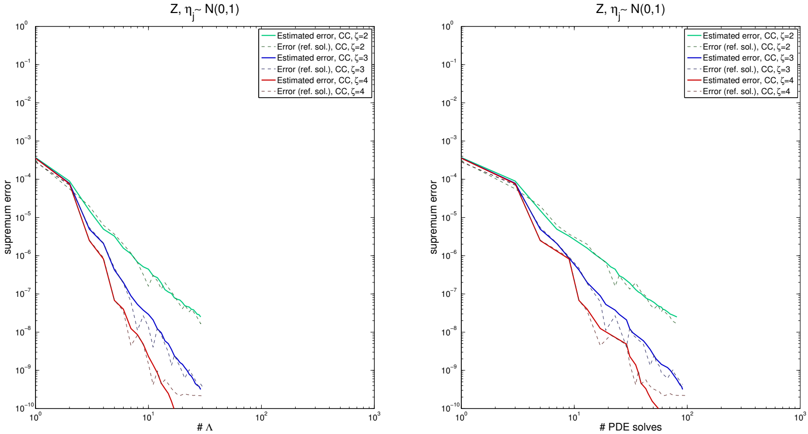
Normalization Constant Z (128 parameters)



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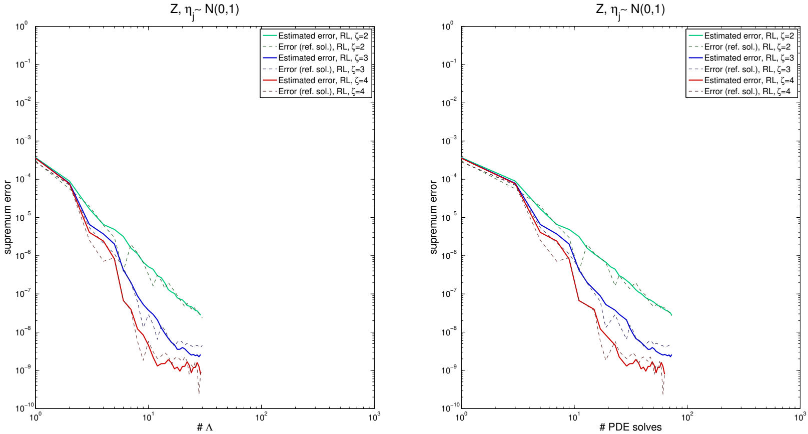
Normalization Constant Z (128 parameters)



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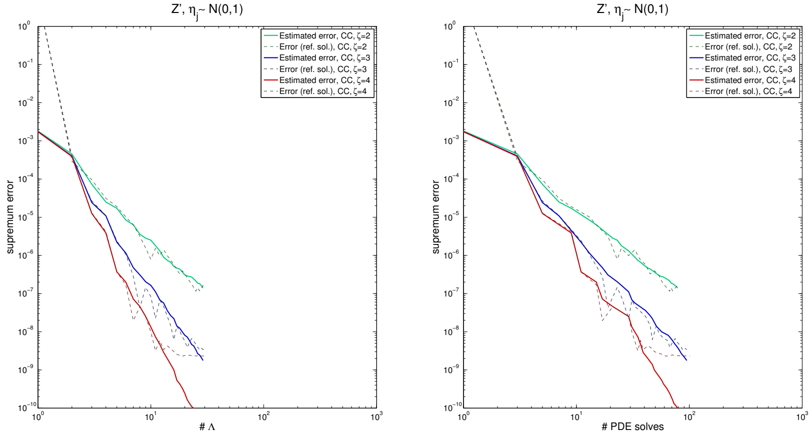
Quantity Z' (128 parameters)



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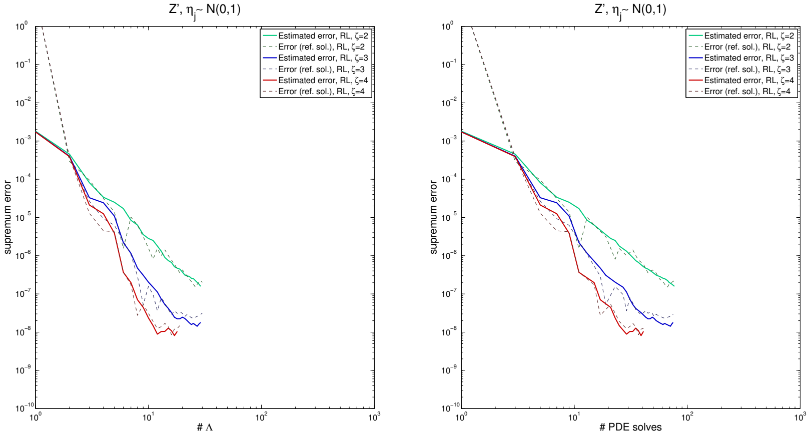

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Numerical Experiments

Model parametric elliptic problem

$$-\text{div}(u\nabla q) = f \quad \text{in } D := [0,1]\,,\; q = 0 \quad \text{in } \partial D\,,$$

with $f(x) = 100 \cdot x$ and

$$\ln(u(x,y)) = \sum_{j=1}^{32} \frac{0.1}{(2j)^{\zeta}} \cos(2j\pi x) y_{2j} + \frac{0.1}{(2j-1)^{\zeta}} \sin((2j-1)\pi x) y_{2j-1}\,,$$

where $y = (y_j)_{j=1,\dots,64}$ are independently normally distributed, ie. $y_j \sim \mathcal{N}(0,1)$, and $\zeta = 2,3,4$.

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
- Uniform mesh with meshwidth $h_D = 2^{-11}$
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Numerical Experiments

Find the unknown data u for given (noisy) data δ,

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- $\mathcal{G} : X \to \mathbb{R}^K$, with $\phi(u) = G(u)$
- $\eta = (\eta_j)_{j=1,\ldots,K}$ iid with $\eta_j \sim \mathcal{N}(0,1)$

Numerical Experiments

Quadrature points

- Gauss-Hermite (GH)

$$\begin{aligned} W(x) &= e^{-x^2}, -\infty < x < \infty \\ H_{j+1} &= 2xH_j - 2jH_{j-1}, \quad H_{-1} = 0, H_0 = 1 \end{aligned}$$

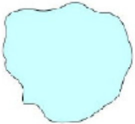
with $n_0 = 1$ and $n_k = 2^k + 1$, for $k \geq 1$

Uncertainty Quantification in Nano Optics

Goal: Quantification of the influence of defects in fabrication process on the optical response of nano structures

- Propagation of plane wave and its interaction with scatterer described by Helmholtz equation (2D).
- Stochastic shape of the scatterer

$$0 < \rho_{\min} \leq \rho(\omega, \phi) \leq \rho_{\max}, \quad \omega \in \Omega, \ \phi \in [0, 2\pi)$$



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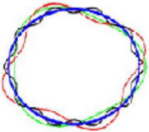
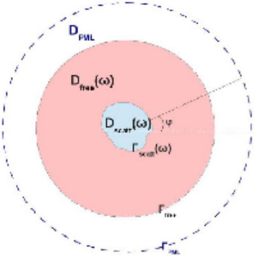
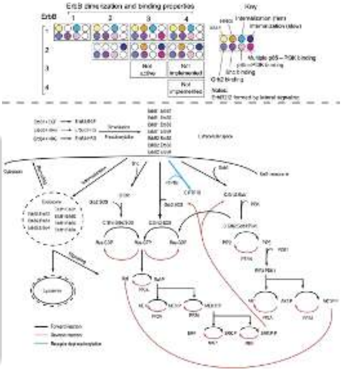




Collaboration with Ralf Hiptmair, Laura Scarabosio

High Dimensional Initial Value Problem

- Mass action models with uncertain reaction rates
- Biochemical reaction pathways with uncertain reaction rate constants
- Chemical reaction cascades with uncertain reaction rate constants

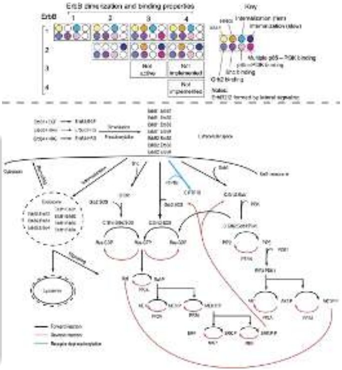


Source: Chen et al., Input-output behavior of ErbB signaling pathways as revealed by a mass action model trained against dynamic data

Goal of computation:
Approximation of system characteristics on the entire, possibly infinite dimensional parameter space

High Dimensional Initial Value Problem

- Mass action models with uncertain reaction rates
- Biochemical reaction pathways with uncertain reaction rate constants
- Chemical reaction cascades with uncertain reaction rate constants



Source: Chen et al.

D-BSSE
Department of Biosystems Science and Engineering

Collaboration with the research group of J. Stelling

High Dimensional Initial Value Problem

Given $x_0(\boldsymbol{y}) \in \mathcal{S}$, $T = [0,1]$, $U = [-1,1]^{\mathbb{N}}$, find $X(t, x_0; \boldsymbol{y}) : T \times \mathcal{S} \times U \to \mathcal{S}$ such that

$$
\begin{aligned}
\frac{\mathrm{d}X}{\mathrm{d}t} &= f(t, X; \boldsymbol{y}) \\
&= f_0(t, X) + \sum_{j \geq 1} y_j f_j(t, X)
\end{aligned}
$$

with $X(0; \boldsymbol{y}) = x_0\,, \;\; 0 \leq t \leq 1\,, \;\; \forall \boldsymbol{y} = (y_j)_{j \geq 1} \in U$

- $\mathcal{S}$ state space (separable and reflexive Banach space)

Affine parameter dependence of the right hand side

Mass action models in computational biology

Stoichiometry with uncertain reaction rate constants

Conclusions and Outlook

- New class of sparse, adaptive quadrature methods for Bayesian inverse problems for a broad class of operator equations
- Dimension-independent convergence rates depending only on the summability of the parametric operator
- Numerical confirmation of the predicted convergence rates

Conclusions and Outlook

- New class of sparse, adaptive quadrature methods for Bayesian inverse problems for a broad class of operator equations
- Dimension-independent convergence rates depending only on the summability of the parametric operator
- Numerical confirmation of the predicted convergence rates

- Gaussian priors and lognormal coefficients
- Adaptive control of the discretization error of the forward problem with respect to the expected significance of its contribution to the Bayesian estimate
- Efficient treatment of large sets of data δ and small observation noise variance Γ

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