Sparsity in Bayesian Inversion of Parametric Operator Equations

Christoph Schwab

joint with Claudia Schillings

Ackn.: A. Cohen, R. DeVore, A. Stuart

June 20, 2013

SAM

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

research supported by the European Research Council under FP7 Grant AdG247277

erc
European Research Council
Established by the European Commission

Outline

Bayesian Inverse Problems (Stuart 2010)

Goal: Expected response in QoI over all uncertain parameters $u \in X$, conditional on noisy data δ

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

- X (separable Banach) space of uncertainties
- $G : X \mapsto \mathcal{X}$ uncertainty-to-solution map
- $\mathcal{O} : \mathcal{X} \mapsto \mathbb{R}^K$ observation operator, $\mathcal{O} \in (\mathcal{X}')^K$
- $\mathcal{G} : X \mapsto \mathbb{R}^K$ uncertainty-to-observation map, $\mathcal{G} = \mathcal{O} \circ G$
- $\eta \in \mathbb{R}^K$ additive observational noise ($\eta \sim \mathcal{N}(0, \Gamma)$), noise (co)variance $\Gamma > 0$.

Linear Operator Equation with operator uncertainty

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

with $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y}')$, $\mathcal{X}$, $\mathcal{Y}$ reflexive Banach spaces, $\mathfrak{a}(v,w) :=_{\mathcal{Y}} \langle w, Av \rangle_{\mathcal{Y}'}$ $\forall v \in \mathcal{X}, w \in \mathcal{Y}$ induced bilinear form; $q(u) = G(u) := (A(u;q))^{-1} f, \ \ \mathcal{G}(u) := \mathcal{O}(G(u))$

Bayesian Inverse Problems (Stuart 2010)

Goal: Expected response in QoI over all uncertain parameters $u \in X$, conditional on noisy data δ

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

- X (separable Banach) space of uncertainties
- $G : X \mapsto \mathcal{X}$ uncertainty-to-solution map
- $\mathcal{O} : \mathcal{X} \mapsto \mathbb{R}^K$ observation operator, $\mathcal{O} \in (\mathcal{X}')^K$
- $\mathcal{G} : X \mapsto \mathbb{R}^K$ uncertainty-to-observation map, $\mathcal{G} = \mathcal{O} \circ G$
- $\eta \in \mathbb{R}^K$ additive observational noise ($\eta \sim \mathcal{N}(0, \Gamma)$), noise (co)variance $\Gamma > 0$.

Bayes LSQ potential $\Phi_\Gamma : \ X \times \mathbb{R}^K \to \mathbb{R}$

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

Bayesian Inverse Problems (Stuart 2010)

Bayes' Theorem:

- Expected value of QoI $\phi(u)$ w.r.t. to posterior measure μ^δ, conditional on given data δ

$$\mathbb{E}^{\mu^\delta}[\phi] = \frac{1}{Z_\Gamma}\int_{u\in X} \exp(-\Phi_\Gamma(u;\delta))\phi(u)d\mu_0(u)$$

Normalization constant $Z_\Gamma = \mathbb{E}^{\mu_0}[\exp(-\Phi_\Gamma(u;\delta))]$.

- μ^δ-expectation over all uncertainties $u \in X$
- Standard Approach: sampling (w.r.t. to unknown measure μ^δ!) MCMC; Rate $\sim \#(\text{PDEsolves})^{-1/2}$

Present work: reformulation of μ^δ-expectation over all $u \in X$ as an infinite dimensional, deterministic quadrature problem; sparsity of integrands; adaptive Smolyak; massively parallel implementation.

Bayesian Inverse Problems (Stuart 2010)

Parametrization of uncertainty $u \in X$ (eg. KL, MRA, ...)

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

- $y = (y_j)_{j \in \mathbb{J}}$ i.i.d sequence of real-valued random variables $y_j \sim \mathcal{U}(-1, 1)$
- $\langle u \rangle, \psi_j \in X, \qquad b_j := \|\psi_j\|_X, \quad (b_j)_{j \geq 1} \in \ell^1(\mathbb{J}),$
- $\mathbb{J}$ finite ($\mathbb{J} = \{1, 2, ..., J\}$) or countably infinite ($\mathbb{J} = \mathbb{N}$) index set

Bayesian prior probability measure on uncertain parameters $\boldsymbol{y}$

$$\mu_0 := \bigotimes_{j \in \mathbb{J}} \pi_j \ , \quad \text{non-gaussian, eg. uniform: } \pi_j = \frac{1}{2} \lambda_1 \ .$$

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

(p, ε) Analyticity (Chkifa, Cohen, DeVore & CS 2012)

$(p, \varepsilon) : 1$ (uniform 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

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

where $U \ni \boldsymbol{y} \mapsto C_0(\boldsymbol{y}) \in L^1(U, \mu_0)$.

$(p, \varepsilon) : 2$ (holomorphy)

There exist $0 \leq p \leq 1$ and $b = (b_j)_{j \in \mathbb{J}} \in \ell^p(\mathbb{J})$ such that for $0 < \varepsilon \leq 1$, there exist $0 < C_\varepsilon < \infty$ and $\rho = (\rho_j)_{j \in \mathbb{J}}$, $\rho_j > 1$ such that

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

and $U \ni \boldsymbol{y} \mapsto q(\boldsymbol{y}) \in \mathcal{X}$ admits holomorphic extension to $\mathcal{E}_\rho := \prod_{j \in \mathbb{J}} \mathcal{E}_{\rho_j} \subset \mathbb{C}^{\mathbb{J}}$

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

(p,ε)-Analyticity $\Longrightarrow$ Sparsity

Theorem (Sparsity)(Chkifa, Cohen, DeVore & CS)

Assume $q(\boldsymbol{y}) = G(u(\boldsymbol{y}))$ is (p,ε)-analytic. Then

- $$\forall \boldsymbol{y} \in U : \quad q(\boldsymbol{y}) = \sum_{\nu\in\mathcal{F}} q_\nu^P \mathcal{P}_\nu(\boldsymbol{y})$$

  with unconditional convergence in $L^\infty(U,\mu_0;\mathcal{X})$, where

  $$\mathcal{P}_\nu(\boldsymbol{y}) := \bigotimes_{j\geq 1} P_{\nu_j}(y_j) \quad \text{(Tensor Legendre Polynomials)}$$

  $$\nu \in \mathcal{F} := (\mathbb{J}\cup\{0\})^{\mathbb{N}}_{finite},\ P_k(1) = 1,\ \|P_k\|_{L^\infty(-1,1)} = 1\ , \quad k = 0,1,\ldots.$$

- There exists sequence of **nested, monotone** $\Lambda_N^P \subset \mathcal{F}$ with $\#(\Lambda_N^P) \leq N$ such that

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

Bayesian Inverse Problem

Bayes' Theorem (parametric; CS & A.M. Stuart 2010)

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

Then μ^δ is a.c. with respect to μ_0:

$$\frac{d\mu^\delta}{d\mu_0}(\boldsymbol{y}) = \frac{1}{Z_\Gamma}\Theta_\Gamma(\boldsymbol{y})$$

with posterior density Θ_Γ given by

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

and normalization constant

$$Z_\Gamma := \int_U \Theta_\Gamma(\boldsymbol{y})d\mu_0(\boldsymbol{y}) \ .$$

Bayesian Inverse Problem

Expectation of *Quantity of Interest (QoI)* $\phi : X \to S$

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

with $Z_\Gamma := \int_{\boldsymbol{y}\in U} \exp(-\frac{1}{2}\big((\delta - \mathcal{G}(u))^\top \Gamma^{-1}(\delta - \mathcal{G}(u))\big)) d\mu_0(\boldsymbol{y}), \quad \Gamma > 0$.

- Reformulation of the forward problem with uncertain, distributed input parameter $u \in X$ as *infinite-dimensional, parametric-deterministic problem*
- Parametric posterior density $\Theta_\Gamma(\boldsymbol{y})$ of μ^δ with respect to the (non-Gaussian) prior μ_0
- Deterministic, adaptive quadrature for Z'_Γ and Z_Γ to compute the posterior expectation of QoI, given data δ

$\Rightarrow$ **Efficient algorithm to approximate expectations conditional on given data with dimension-independent rates of convergence** $> 1/2$

Sparsity of the Posterior Density

Theorem (Cl. Schillings and CS 2013)

Assume that the forward solution map $U \ni \boldsymbol{y} \mapsto q(\boldsymbol{y})$ is (p, ε)-analytic for some $0 < p < 1$ and $\varepsilon > 0$.
Then the Bayesian posterior density $\Theta_\Gamma(\boldsymbol{y})$ is, as a function of the parameter $\boldsymbol{y}$, likewise (p, ε)-analytic and, therefore, p-sparse.

Examples:

- affine-parametric, linear operator equations
- semilinear elliptic PDEs (Hansen & CS; Math. Nachr. 2013)
- parametric initial value ODEs
  (Hansen & CS; Vietnam J. Math. 2013)
- elliptic multiscale problems
  (Hoang & CS; Analysis and Applications 2012)

N-term Approximation Rates

Theorem (Cl. Schillings and CS 2013)

Assume that the uncertainty-to-observation map $\mathcal{G}(u(\boldsymbol{y})) : U \mapsto \mathbb{R}^K$ is (p, ε)-analytic for some $0 < p < 1$.
Then exists a nested sequence $(\Lambda_N^\Theta)_{N\geq 1} \subset \mathcal{F}$ of monotone sets $\Lambda_N^\Theta \subset \mathcal{F}$ such that $\#(\Lambda_N^\Theta) \leq N$ and such that, for all N,

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

Evaluation of $\mathbb{E}^{\mu^\delta}[\phi]$ by Adaptive Smolyak quadrature algorithm with convergence rate $N^{-(1/p-1)}$ (N = # PDE solves).
Λ_N^P = ? **Either** direct construction from sets Λ_N^G in adaptive sGFEM (CS & Stuart (2010)), **or b) adaptive Smolyak** or ...

Smolyak: Univariate Quadratures

Family of univariate quadratures (for coordinate measures)

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

with $\mathrm{g} : [-1, 1] \mapsto \mathcal{S}$ for state space $\mathcal{S}$

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

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

Smolyak: Univariate Quadratures

Family of univariate quadratures (for coordinate measures)

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

with $\mathrm{g} : [-1,1] \mapsto \mathcal{S}$ for state space $\mathcal{S}$

- $(Q^k)_{k\geq 0}$ 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

Univariate quadrature difference operator

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

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

Smolyak: Univariate Quadratures

Family of univariate quadratures (for coordinate measures)

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

with $\mathrm{g} : [-1,1] \mapsto \mathcal{S}$ for state space $\mathcal{S}$

- $(Q^k)_{k\geq 0}$ 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

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

Smolyak: Tensorization

Tensorized multivariate quadrature 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 collocation points $\mathcal{Z}^\nu = \times_{j\geq 1}\mathcal{Z}^{\nu_j} \subset U$

- 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 Smolyak Quadrature Operator

For any finite monotone set $\Lambda \subset \mathcal{F}$, Q_Λ 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 Smolyak grid $\mathcal{Z}_\Lambda = \cup_{\nu \in \Lambda} \mathcal{Z}^\nu$

Theorem (Cl. Schillings and CS 2013)

For any finite monotone index set $\Lambda_N \subset \mathcal{F}$, the sparse quadrature $\mathcal{Q}_{\Lambda_N}$ is exact for any polynomial $g \in \mathbb{P}_{\Lambda_N}$, i.e. it holds

$$\mathcal{Q}_{\Lambda_N}(g) = I(g), \qquad \forall g \in \mathbb{S}_{\Lambda_N} := \mathbb{P}_{\Lambda_N} \otimes \mathcal{S}\,,$$

with $\mathbb{P}_{\Lambda_N} = \mathrm{span}\{y^\nu : \nu \in \Lambda_N\}$, i.e. $\mathbb{S}_{\Lambda_N} = \mathrm{span}\left\{\sum_{\nu \in \Lambda_N} s_\nu y^\nu : s_\nu \in \mathcal{S}\right\}$, and $I(g) = \int_U g(\boldsymbol{y}) \mu_0(d\boldsymbol{y})$.

Convergence Rates for Adaptive Smolyak Integration

Corollary (Cl. Schillings and CS 2013)

Assume that the forward solution map $U \ni \boldsymbol{y} \mapsto q(\boldsymbol{y})$ is (p, ε)-analytic for some $0 < p < 1$ and $\varepsilon > 0$.

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

$$|Z_\Gamma - \mathcal{Q}_{\Lambda_N}[\Theta_\Gamma]| \leq C^1(\Gamma, p) N^{-s} ,$$

with $s = 1/p - 1$, and, for $\Psi_\Gamma(\boldsymbol{y}) := \Theta_\Gamma(\boldsymbol{y})\phi(u(\boldsymbol{y}))$,

$$\|Z'_\Gamma - \mathcal{Q}_{\Lambda_N}[\Psi_\Gamma]\|_{\mathcal{S}} \leq C^2(\Gamma, p) N^{-s} \ .$$

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

Remark: *SAME* index set Λ_N for *BOTH*, Z_Γ and Z'_Γ.

Convergence Rates for Adaptive Smolyak Integration

Remark: *SAME* index set Λ_N for *BOTH*, Z_Γ and Z'_Γ.

Sketch of proof

- Relating the quadrature error with Legendre gpc coefficients

$$|I[\Theta_\Gamma] - \mathcal{Q}_\Lambda[\Theta_\Gamma]| \leq 2 \cdot \sum_{\nu \notin \Lambda} \gamma_\nu |\theta_\nu^P|$$

  and

$$\|I[\Psi_\Gamma] - \mathcal{Q}_\Lambda[\Psi_\Gamma]\|_{\mathcal{S}} \leq 2 \cdot \sum_{\nu \notin \Lambda} \gamma_\nu \|\psi_\nu^P\|_{\mathcal{S}}$$

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

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

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

Adaptive Construction of $\{\Lambda_N\}_{N\geq 1}$

Successive identification of N largest Smolyak contributions

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

A. Chkifa, A. Cohen and Ch. Schwab. High-dimensional adaptive sparse polynomial interpolation and applications to parametric PDEs, JFoCM 2013.

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

Adaptive Construction of $\{\Lambda_N\}_{N\geq 1}$

function ASG
    Set $\Lambda_1 = \{0\}\,, k = 1$ and compute $\Delta_0(\Theta)$.
    Determine the set of reduced 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**
        Pick ν from $\mathcal{N}(\Lambda_k)$ w. largest $|\Delta_\nu|$ and set $\Lambda_{k+1} := \Lambda_k \cup \{\nu\}$.
        Determine the set of reduced 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 $\alpha_j = \frac{1.8}{j^\zeta}$, $\zeta = 2,3,4$.

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
- Uniform mesh with meshwidth $h_T = h_D = 2^{-10}$
- LAPACK's DPTSV routine

Numerical Experiments

Find the expected system response, given (noisy) data

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

Expectation of interest Z'_Γ / Z_Γ

$$\begin{aligned} Z'_\Gamma &= \int_U \exp\big(-\Phi_\Gamma(u;\delta)\big)\,\phi(u)\Big|_{u=\langle u\rangle+\sum_{j=1}^{64} y_j\psi_j} d\mu_0(\boldsymbol{y}) \\ Z_\Gamma &= \int_U \exp\big(-\Phi_\Gamma(u;\delta)\big)\Big|_{u=\langle u\rangle+\sum_{j=1}^{64} y_j\psi_j} d\mu_0(\boldsymbol{y}) \end{aligned}$$

- 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 $K = 1,\ N_{K,D} = 1, N_{K,T} = 1,\ K = 3,\ N_{K,D} = 2, N_{K,T} = 1,\ K = 9,\ N_{K,D} = 2, N_{K,T} = 2$
- $\mathcal{G} : L^\infty(D) \to \mathbb{R}^K$, with $K = 1, 3, 9$, $\phi(u) = G(u)$
- $\eta = (\eta_j)_{j=1,\dots,K}$ iid with $\eta_j \sim \mathcal{N}(0,1)$, $\eta_j \sim \mathcal{N}(0, 0.5^2)$ and $\eta_j \sim \mathcal{N}(0, 0.1^2)$

Posterior Expectation of QoI Z'_Γ

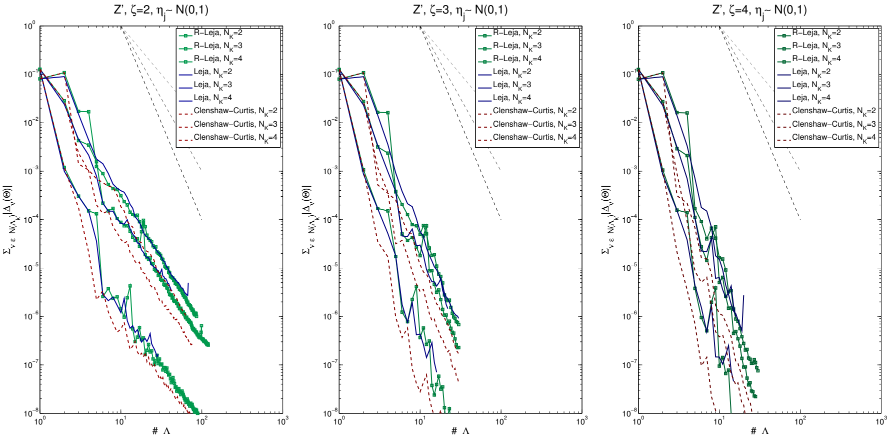

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0,1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

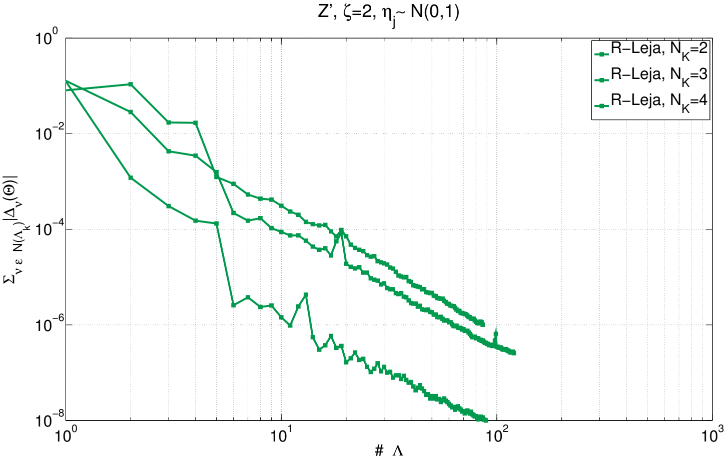

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

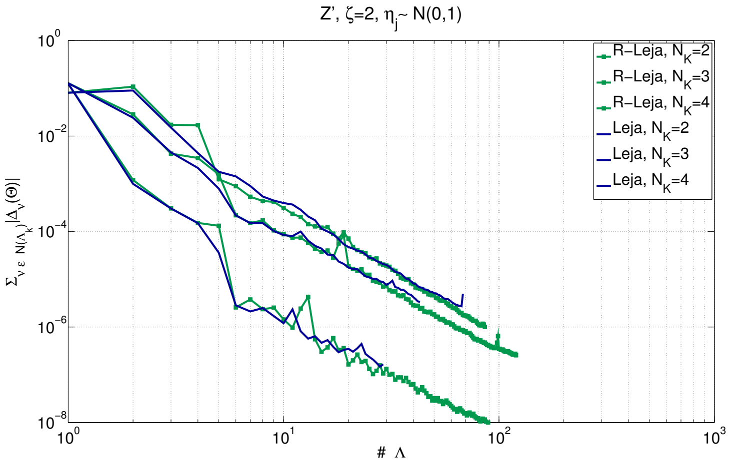

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9,\ \eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

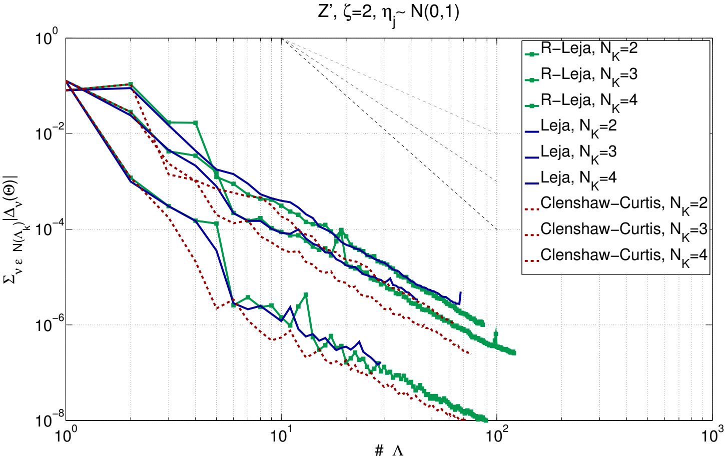

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

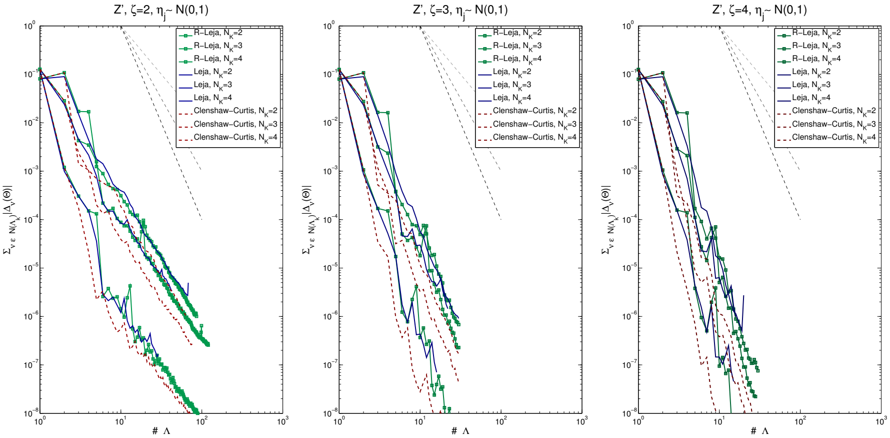

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0,1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

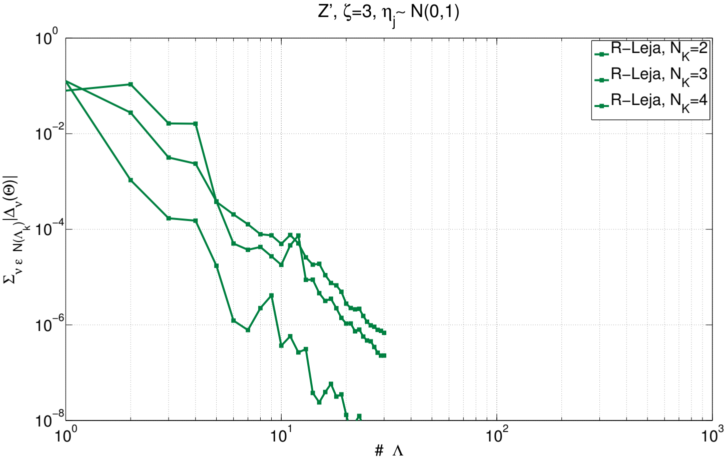

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9,\ \eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

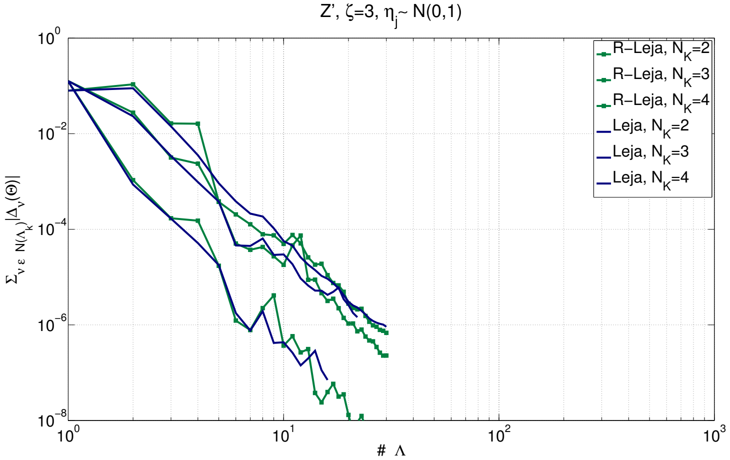

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0,1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

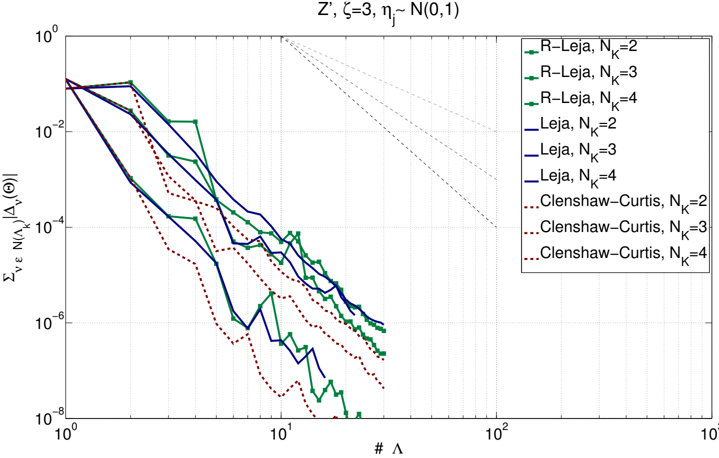

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0,1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

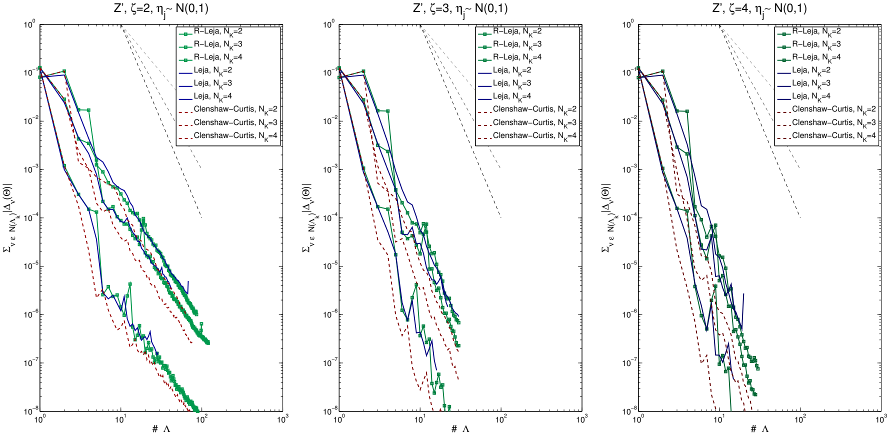

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

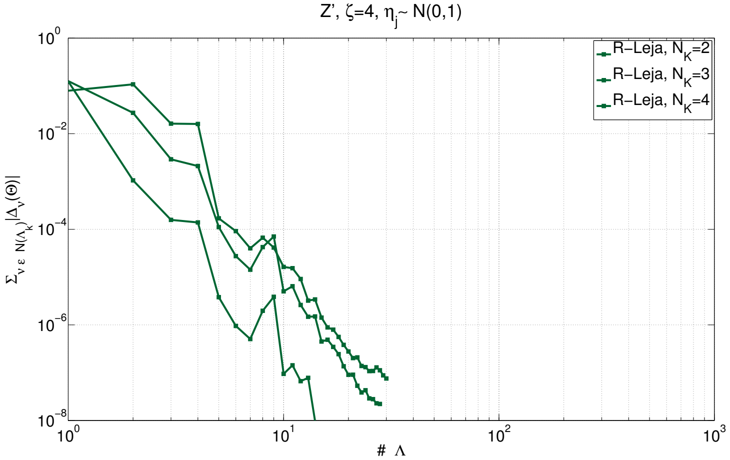

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0,1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

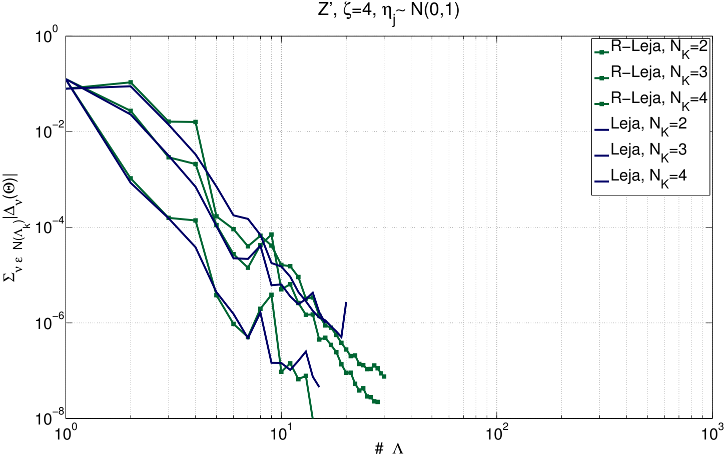

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

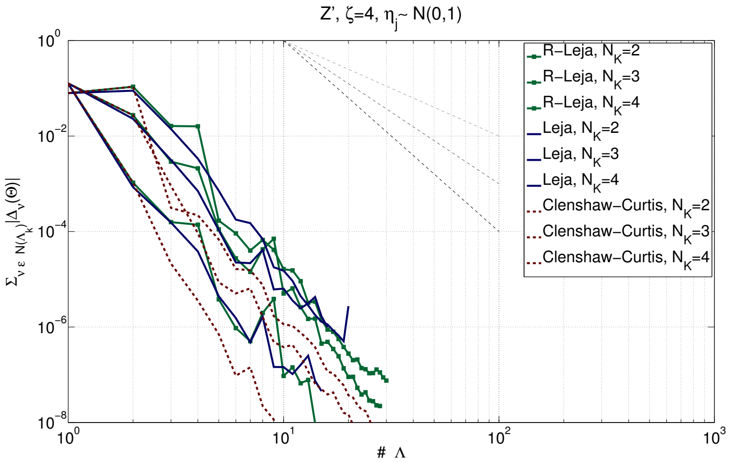

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9,\ \eta \sim \mathcal{N}(0,1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

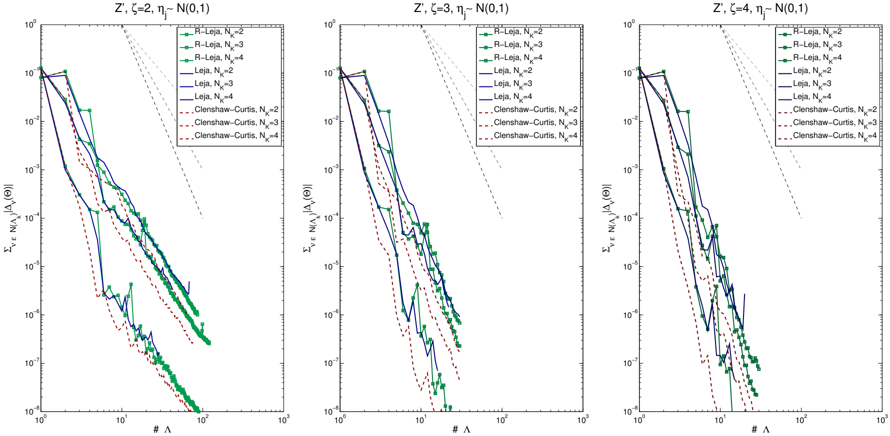

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

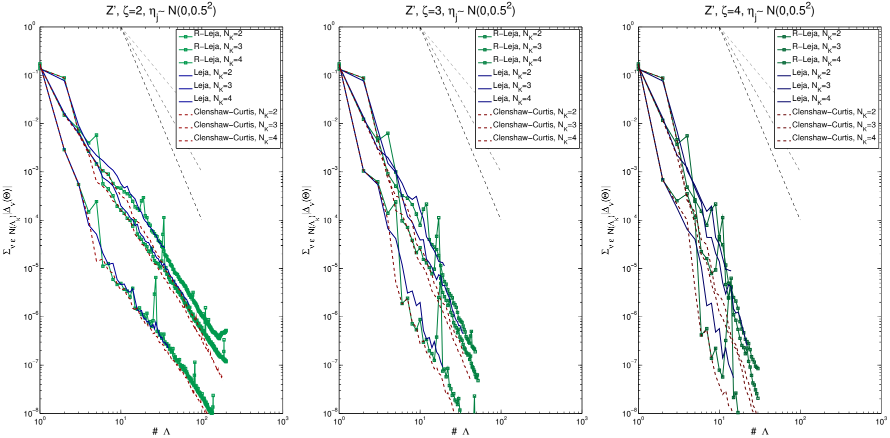

Figure: Comparison of the error curves of the Posterior Expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 0.5^2)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

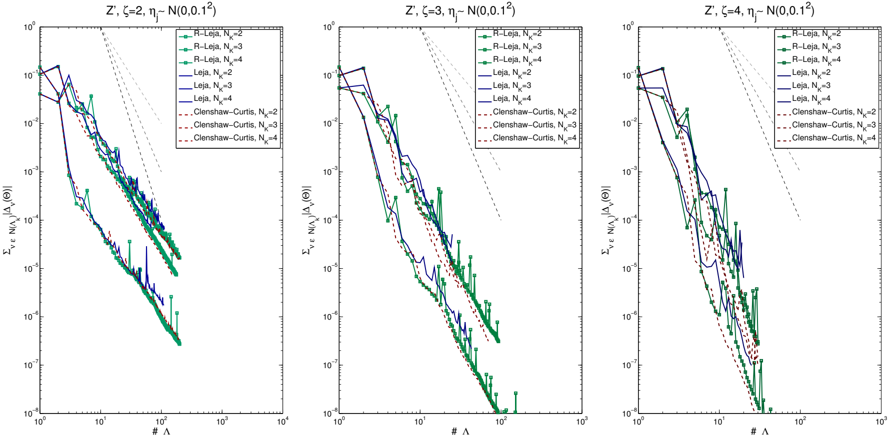

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1,3,9,\ \eta \sim \mathcal{N}(0, 0.1^2)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

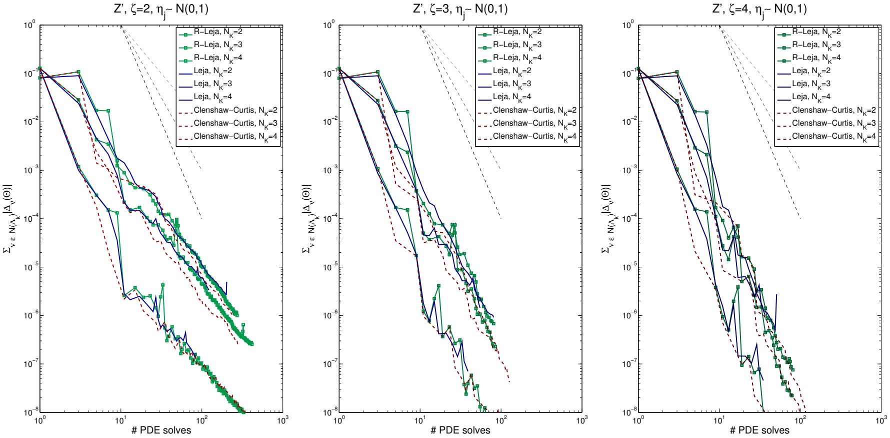

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ with respect to the number of PDE solves needed based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

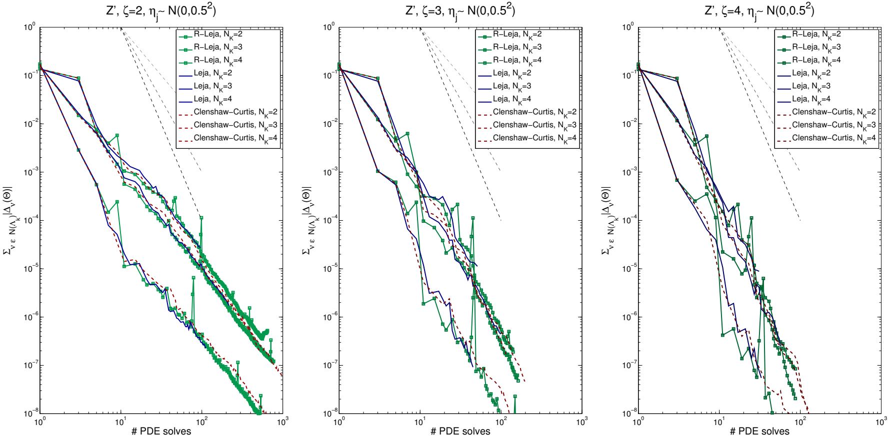

Figure: Comparison of the error curves of the posterior expectation of QoI Z'_Γ with respect to the number of PDE solves needed based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 0.5^2)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'_Γ

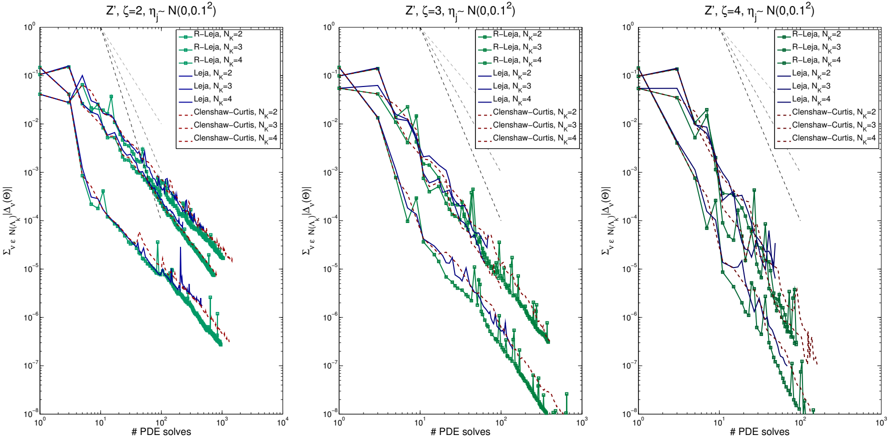

Figure: Comparison of the error curves of the Posterior Expectation of QoI Z'_Γ with respect to the number of PDE solves needed based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 0.1^2)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'

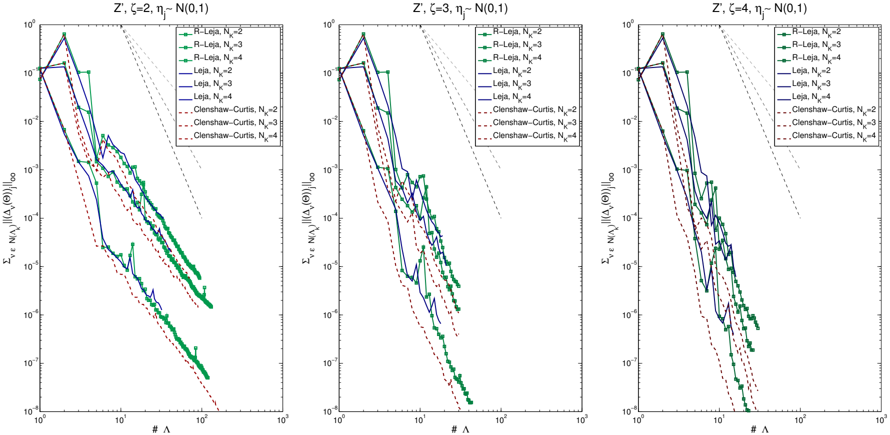

Figure: Comparison of the L^∞ error curves of QoI Z' with respect to the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1$, $K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 1)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'

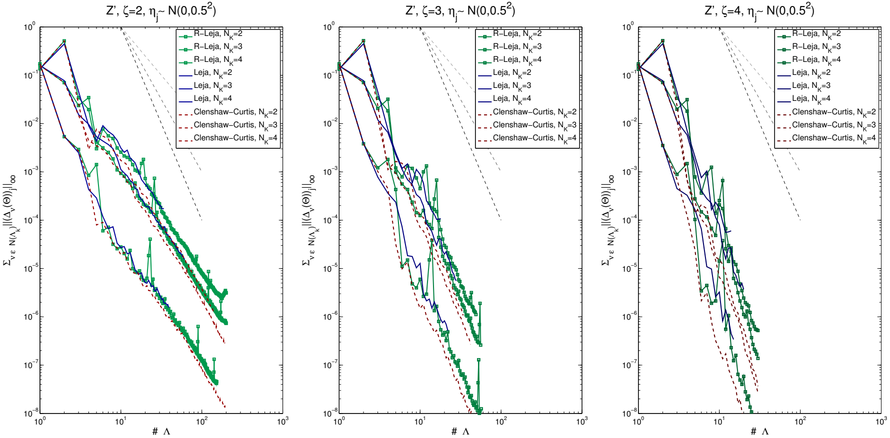

Figure: Comparison of the L^∞ error curves of QoI Z' with respect to cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 0.5^2)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Posterior Expectation of QoI Z'

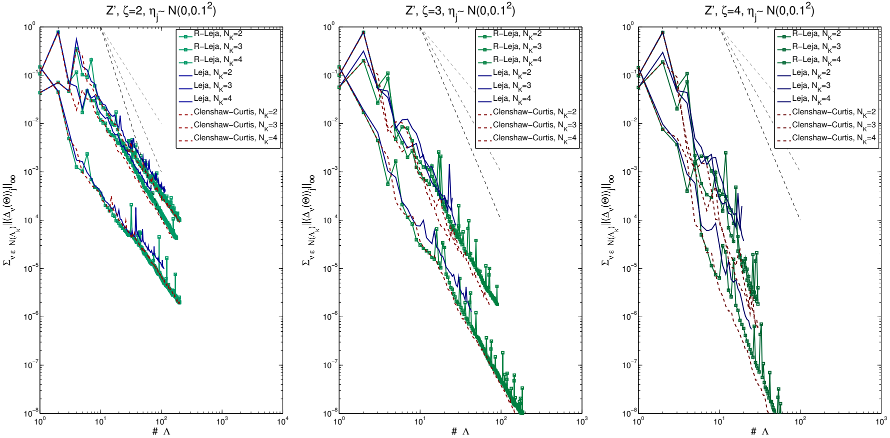

Figure: Comparison of the L^∞ error curves of QoI Z' with respect to the cardinality of the index set Λ_N based on the sequences CC, L and RL with $K = 2^{N_K} - 1\,,\ K = 1, 3, 9$, $\eta \sim \mathcal{N}(0, 0.1^2)$ and $\zeta = 2$ (l.), $\zeta = 3$ (m.) and $\zeta = 4$ (r.).

Conclusions and Outlook

- **deterministic, gpc-based data-adaptive quadrature** for Bayesian inversion and estimation problems for **parametric operator equations with distributed uncertainty** u
- Dimension-independent convergence bound $C_\Gamma N^{-s}$
- Γ independent **rate** $s = 1/p - 1 > 1/2, \quad N = \#$ PDE-solves
- Γ dependent **constant** $C_\Gamma \sim C \exp(-b/\Gamma)$, $b, C > 0$ ind. of Γ
- $\Gamma \downarrow 0$? Asymptotic Expansion

$$\mathbb{E}^{\mu^\delta}[\phi(u)] = \frac{Z'_\Gamma}{Z_\Gamma} \sim \sum_{k \geq 0} a_k \Gamma^k \quad \text{as} \quad \Gamma \downarrow 0$$

$\Longrightarrow$ Richardson-Extrapolation w.r.t. to $\Gamma \downarrow 0$ (SC & Schillings'13)

Conclusions and Outlook

- **deterministic, gpc-based data-adaptive quadrature** for Bayesian inversion and estimation problems for **parametric operator equations with distributed uncertainty** u
- Dimension-independent convergence bound $C_\Gamma N^{-s}$
- Γ independent **rate** $s = 1/p - 1 > 1/2, \quad N = \#$ PDE-solves
- Γ dependent **constant** $C_\Gamma \sim C \exp(-b/\Gamma)$, $b, C > 0$ ind. of Γ
- $\Gamma \downarrow 0$? Asymptotic Expansion

$$\mathbb{E}^{\mu^\delta}[\phi(u)] = \frac{Z'_\Gamma}{Z_\Gamma} \sim \sum_{k \geq 0} a_k \Gamma^k \quad \text{as} \quad \Gamma \downarrow 0$$

$\Longrightarrow$ Richardson-Extrapolation w.r. to $\Gamma \downarrow 0$ (SC & Schillings'13)

- Adaptive control of the discretization error of the forward problem with respect to significance in Smolyak detail $\Delta_\nu[\Psi_\Gamma]$
- No MCMC burn-in

References

- Calvi J-P and Phung Van M 2011 On the Lebesgue constant of Leja sequences for the unit disk and its applications to multivariate interpolation *Journal of Approximation Theory* **163** 608-622
- Calvi J-P and Phung Van M 2012 Lagrange interpolation at real projections of Leja sequences for the unit disk *Proceedings of the American Mathematical Society* **140** 4271–4284
- CHKIFA A 2013 On the Lebesgue constant of Leja sequences for the unit disk *Journal of Approximation Theory* **166** 176-200
- Chkifa A, Cohen A and Schwab C 2013 High-dimensional adaptive sparse polynomial interpolation and applications to parametric PDEs JFoCM 2013
- Cohen A, DeVore R and Schwab C 2011 Analytic regularity and polynomial approximation of parametric and stochastic elliptic PDEs *Analysis and Applications* **9** 1-37
- Gerstner T and Griebel M 2003 Dimension-adaptive tensor-product quadrature *Computing* **71** 65-87
- Hansen M and Schwab C 2013 Sparse adaptive approximation of high dimensional parametric initial value problems *Vietnam J. Math.* **1** 1-35
- Hansen M, Schillings C and Schwab C 2012 Sparse approximation algorithms for high dimensional parametric initial value problems *Proceedings 5th Conf. High Performance Computing, Hanoi*(Springer LNCSE 2013)
- Schillings C and Schwab C 2013 Sparse, adaptive Smolyak algorithms for Bayesian inverse problems (*Inverse Problems*)
- Schwab C and Stuart A M 2012 Sparse deterministic approximation of Bayesian inverse problems *Inverse Problems* **28** 045003

Thank you for your attention & comments

Postdoctoral Fellowships
www.sam.math.ethz.ch