Analysis of the stability and accuracy of discrete least-squares approximation on multivariate polynomial spaces†

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Outline

Notation and definitions

For any $d \geq 1$ define $\Gamma := [-1,1]^d$, $N \subseteq \mathbb{R}$.

$(\Gamma \times N, \Sigma, w)$ complete probability space with Σ being the σ-algebra of Borel sets and w being a probability measure.

$$(y,\eta) \sim w, \quad \mathrm{supp}(y) = \Gamma, \quad \mathrm{supp}(\eta) = N.$$

μ marginal probability measure w.r.t. y.

Assumption: μ absolutely continuous w.r.t. Lebegue measure λ on Γ.

$\rho : \Gamma \to \mathbb{R}^+, \rho = d\mu/d\lambda$ probability density function associated to μ.

From now on, given the real parameters $\alpha, \beta > -1$:

$$\rho(y) := \mathcal{B}(\alpha,\beta)^{-d} \prod_{i=1}^{d} (1-y_i)^\alpha (1+y_i)^\beta, \quad y \in \Gamma.$$

Notation and definitions

$$\langle f_1, f_2 \rangle_{L^2_\rho(\Gamma)} := \int_\Gamma f_1(y) f_2(y) \rho(y) dy, \quad \langle f_1, f_2 \rangle_M := \frac{1}{M} \sum_{m=1}^{M} f_1(y_m)\, f_2(y_m),$$

$$\| \cdot \|_{L^2_\rho} := \langle \cdot, \cdot \rangle_{L^2_\rho}^{1/2}, \quad \| \cdot \|_M := \langle \cdot, \cdot \rangle_M^{1/2},$$

with $y_1, \dots, y_M$ being any points in Γ.

Given univariate L^2_ρ-orthonormal polynomials $(\varphi_k)_{k \geq 0}$ and a multi-index set $\Lambda \subset \mathbb{N}_0^d$, for any $\nu \in \Lambda$ we define

$$\psi_\nu(y) := \prod_{i=1}^{d} \varphi_{\nu_i}(y_i), \quad y \in \Gamma,$$

$$\mathbb{P}_\Lambda := \mathrm{span}\left\{ \psi_\nu : \nu \in \Lambda \right\}.$$

Observation models

We wish to approximate $\phi : \Gamma \to \mathbb{R}$ in the L^2 sense, using pointwise evaluations $\phi(y_1), \ldots, \phi(y_M)$ in M points $y_1, \ldots, y_M \in \Gamma$.

Observation models:

$$\text{noiseless observation model:} \qquad z_i = \phi(y_i), \ \ i = 1, \ldots, M,$$
$$\text{noisy observation model:} \qquad z_i = \phi(y_i) + \eta_i, \ \ i = 1, \ldots, M,$$

$(y_1, \eta_1), \ldots, (y_M, \eta_M)$ are i.i.d. w.r.t. the measure w, BUT $\eta_i = \eta(y_i)$.

Discrete least squares on polynomial spaces

We define the continuous and discrete L^2 projections of f over $\mathbb{P}_\Lambda$ as

$$\Pi_\Lambda f := \operatorname*{argmin}_{v \in \mathbb{P}_\Lambda} \|f - v\|_{L^2_\rho}, \qquad \Pi_\Lambda^M f := \operatorname*{argmin}_{v \in \mathbb{P}_\Lambda} \|f - v\|_M.$$

Algebraic formulation: design matrix $[D]_{ij} = \psi_j(y_i)$, right-hand side $[b]_i = f(y_i)$, for any $i = 1, \dots, M$ and $j = 1, \dots, \#\Lambda$.

Normal equations:

$$D^\top D \, \boldsymbol{\beta} = D^\top b,$$

with $\boldsymbol{\beta}$ containing the coefficients of the expansion $\Pi_\Lambda^M \phi = \sum_{\nu \in \Lambda} \beta_\nu \psi_\nu$.

We define also the matrices $G := D^\top D / M$ and $J = D/M$ such that

$$G\boldsymbol{\beta} = J^\top b.$$

Stability and accuracy of DLS on poly. spaces

Random points , **density bounded support** , **noiseless obs.**

Cohen, Davenport, Leviatan, FoCM 2013,
M., Nobile, von Schwerin, Tempone, FoCM 2014,
Chkifa, Cohen, M., Nobile, Tempone, M2AN 2015.

Low-discrepancy points , **density bounded support** , **noiseless obs.**

Zhou, Narayan, Xu, SISC 2014,
M., Nobile, J.Complexity 2015.

Random points , **Gaussian density** , **noiseless obs.**

Tang, Zhou, SISC 2014.

Random points , **density bounded support** , **noisy obs.**

Cohen, Davenport, Leviatan FoCM 2013,
Chkifa, Cohen, M., Nobile, Tempone, M2AN 2015,
M., Nobile, Tempone, JMA 2015.

2015 - onwards: many other directions of analysis (weighted least squares, relation with ℓ_1 minimization, change of orthonormal basis, . . .)

Optimality of discrete least squares in the L^2_ρ norm

In any dimension, with any index set Λ and any ρ with bounded support:

Proposition (M., Nobile, von Schwerin and Tempone, FoCM 2014)

For any (random or deterministic) choice of M points in Γ it holds

$$\|\phi - \Pi_\Lambda^M \phi\|_{L^2_\rho} \leq \left(1 + \sqrt{|||G^{-1}|||}\right) \inf_{v \in \mathbb{P}_\Lambda} \|\phi - v\|_{L^\infty}.$$

Proof

Theorem (M., Nobile, von Schwerin and Tempone, FoCM 2014)

Given M points in Γ, being realizations of random variables independent and identically distributed w.r.t. ρ, it holds

$$\lim_{M \to +\infty} |||G^{-1}||| = \lim_{M \to +\infty} |||G||| = 1, \quad \textit{almost surely}.$$

Proposition (M., Nobile, von Schwerin and Tempone, FoCM 2014)

$$cond(G) = |||G|||\ |||G^{-1}|||.$$

Markov and Nikolskii inequalities for multivariate polynomials with downward closed multi-index sets

Definition (Downward closed multi-index set)

Λ is downward closed if $(\boldsymbol{\nu} \in \Lambda \quad \text{and} \quad \boldsymbol{\nu}' \leq \boldsymbol{\nu}) \Rightarrow \boldsymbol{\nu}' \in \Lambda$.

Lemma (M., J.Approx.Theory 2015)

In any dimension, for any Λ downward closed and any $\alpha, \beta \in \mathbb{N}_0$ it holds

$$\|v\|^2_{L^\infty(\Gamma)} \leq (\#\Lambda)^{2\max\{\alpha,\beta\}+2} \|v\|^2_{L^2_\rho(\Gamma)}, \quad \forall v \in \mathbb{P}_\Lambda(\Gamma).$$

Lemma (M., J.Approx.Theory 2015)

In any dimension and for any Λ downward closed, when $\alpha = \beta = 0$ (Legendre polynomials), it holds

$$\left\| \frac{\partial^d}{\partial y_1 \cdots \partial y_d} v \right\|^2_{L^2_\rho(\Gamma)} \leq 4^{-d} (\#\Lambda)^4 \|v\|^2_{L^2_\rho(\Gamma)}, \quad \forall v \in \mathbb{P}_\Lambda(\Gamma).$$

Assume that $|\phi| \leq \tau$ almost surely w.r.t. ρ and define

$$T_\tau(t) := \mathrm{sign}(t)\min\{\tau, |t|\}, \qquad \widetilde{\Pi}_\Lambda^M := T_\tau(\Pi_\Lambda^M).$$

Theorem (Chkifa, Cohen, M., Nobile and Tempone, M2AN 2015)

For any $\gamma>0$ and any downward closed Λ, if M is such that

$$\frac{0.15}{1+\gamma}\frac{M}{\ln M} \geq \begin{cases} (\#\Lambda)^{\ln 3/\ln 2}, & \text{if} \quad \alpha=\beta=-1/2, \\ (\#\Lambda)^{2\max\{\alpha,\beta\}+2}, & \text{if} \quad \alpha,\beta\in\mathbb{N}_0, \end{cases}$$

then, for any $\phi \in L^\infty(\Gamma)$ with $\|\phi\|_{L^\infty} \leq \tau$, it holds that

$$Pr(cond(G) \leq 3) \geq 1-2M^{-\gamma},$$

$$Pr\left(\|\phi - \Pi_\Lambda^M\phi\|_{L^2_\rho} \leq (1+\sqrt{2})\inf_{v\in\mathbb{P}_\Lambda}\|\phi - v\|_{L^\infty}\right) \geq 1-2M^{-\gamma},$$

$$\mathbb{E}\left(\|\phi - \widetilde{\Pi}_\Lambda^M\phi\|^2_{L^2_\rho}\right) \leq \left(1+\frac{0.6}{(1+\gamma)\ln M}\right)\|\phi - \Pi_\Lambda\phi\|^2_{L^2_\rho} + 8\tau^2M^{-\gamma}.$$

($\delta = 1/2$ everywhere!)

Assumptions on the type of noise

Conditional mean of the noise (noise offset) $\overline{\eta}(y) := \mathbb{E}(\eta|y)$.

Fluctuations of the noise $\widetilde{\eta} := \eta - \overline{\eta}$.

Noise offset square-integrable: $\|\overline{\eta}\|_{L^2_\rho} < +\infty, \qquad (\|\overline{\eta}\|^2_{L^2_\rho} = \mathbb{E}(\overline{\eta}^2))$.

Noise has uniformly bounded conditional variance

$$\sigma^2 := \max_{y\in\Gamma} \mathbb{E}\left(|\eta - \overline{\eta}(y)|^2 y\right) < +\infty.$$

unbounded noise model $\mathrm{Im}(\eta_i) = \mathbb{R}, \forall i, \quad \|\overline{\eta}\|_{L^2_\rho} < +\infty, \quad \sigma^2 < +\infty.$

bounded noise model $\|\widetilde{\eta}\|_{L^\infty} < +\infty, \quad \|\overline{\eta}\|_{L^\infty} < +\infty.$

Theorem (M.,Nobile,Tempone, J. Multivariate Analysis 2015)

For any $\gamma > 0$ *and any downward closed* Λ, *if* M *is such that*

$$\frac{0.15}{1+\gamma}\frac{M}{\ln M} \geq \begin{cases} (\#\Lambda)^{\ln 3/\ln 2}, & \textit{if} \quad \alpha=\beta=-1/2, \\ (\#\Lambda)^{2\max\{\alpha,\beta\}+2}, & \textit{if} \quad \alpha,\beta \in \mathbb{N}_0, \end{cases}$$

then, for any $\phi \in L^\infty(\Gamma)$ *with* $\|\phi\|_{L^\infty} \leq \tau$, *it holds that:*
with the *bounded noise model*

$$Pr\Bigg(\|\phi - \Pi_\Lambda^M(\phi+\eta)\|^2_{L^2_\rho} \leq 5 \inf_{v\in\mathbb{P}_\Lambda} \|\phi - v\|^2_{L^\infty} + 3\widetilde{\eta}^2_{max}(1+\gamma)\ln M \frac{\#\Lambda}{M} + 24\overline{\eta}^2_{max} \Bigg) \geq 1 - 2M^{-\gamma},$$

with the *unbounded noise model*

$$\mathbb{E}\left(\|\phi - \widetilde{\Pi}_\Lambda^M(\phi+\eta)\|^2_{L^2_\rho} \right) \leq \left(1 + \frac{1.2}{(1+\gamma)\ln M} \right) \|\phi - \Pi_\Lambda \phi\|^2_{L^2_\rho} + \frac{8\,\sigma^2\#\Lambda}{M} + \|\overline{\eta}\|^2 \left(8 + \frac{1.2}{(1+\gamma)\ln M} \right) + 8\tau^2 M^{-\gamma}.$$

Sketch of the proof (poster also available)

For any $\delta \in (0,1)$ define the event

$$\Omega_\delta^M := \left\{ (y,\eta) \in \Omega^M := \Omega \times \ldots \times \Omega \ : \ |||G(y) - I||| \leq \delta \right\} \in \Sigma^M := \prod_{i=1}^{M} \Sigma_i .$$

$$[\mathbf{g}]_j := \phi(y_j) - (\Pi_\Lambda \phi)(y_j), \quad [\overline{\boldsymbol{\eta}}]_j := \overline{\boldsymbol{\eta}}(y_j), \quad [\widetilde{\boldsymbol{\eta}}]_j := \widetilde{\boldsymbol{\eta}}(y_j), \quad j = 1, \ldots, M.$$

$$z_\Lambda := \Pi_\Lambda^M(\phi + \eta), \quad e_n(\phi)^2 := \|\phi - \Pi_\Lambda \phi\|^2_{L^2_\rho}.$$

On the event Ω_δ^M it holds that

$$\begin{aligned}
\|\phi - z_\Lambda\|^2 &\leq \|\phi - \Pi_\Lambda \phi\|^2 + 2\|\Pi_\Lambda^M(\phi - \Pi_\Lambda\phi)\|^2 + 2\|\Pi_\Lambda^M \phi - z_\Lambda\|^2 \\
&= e_n(\phi)^2 + 2\|G^{-1}J^\top \mathbf{g}\|^2_{\ell^2} + 2\|G^{-1}J^\top \boldsymbol{\eta}\|^2_{\ell^2} \\
&\leq e_n(\phi)^2 + 2(1-\delta)^{-2}\|J^\top \mathbf{g}\|^2_{\ell^2} + 2(1-\delta)^{-2}\|J^\top \boldsymbol{\eta}\|^2_{\ell^2} \\
&\leq e_n(\phi)^2 + 2(1-\delta)^{-2}\|J^\top \mathbf{g}\|^2_{\ell^2} + 4(1-\delta)^{-2}\left(\|J^\top \overline{\boldsymbol{\eta}}\|^2_{\ell^2} + \|J^\top \widetilde{\boldsymbol{\eta}}\|^2_{\ell^2}\right)
\end{aligned}$$

Sketch of the proof

Theorem (M., Nobile, Tempone, J. Multivariate Analysis 2015)

For any $\gamma > 0$, any $\delta \in (0,1)$, any Λ downward closed and any M satisfying

$$\frac{0.15}{1+\gamma}\frac{M}{\ln M} \geq \begin{cases} (\#\Lambda)^{\ln 3/\ln 2}, & \textit{if} \quad \alpha = \beta = -1/2, \\ (\#\Lambda)^{2\max\{\alpha,\beta\}+2}, & \textit{if} \quad \alpha,\beta \in \mathbb{N}_0, \end{cases}$$

with the bounded noise model it holds that

$$Pr\left(\|J^\top \widetilde{\boldsymbol{\eta}}\|_{\ell^2}^2 > 2(1+\gamma)(1+\delta)\frac{\widetilde{\eta}_{max}^2 \, \#\Lambda \ \ln M}{M} \mid \Omega_\delta^M \right) \leq 2M^{-\gamma}.$$

Proof: probability union bounds + Hoeffding's inequality (the random variables in $\widetilde{\boldsymbol{\eta}}$ have zeromean!).

Discrete least squares with deterministic points: the multivariate case with uniform density in $[0,1]^d$

Let $t \geq 0$, $m \geq 1$, $d \geq 1$ and $b \geq 2$ be integers with $t \leq m$.

A (t, m, d)-net in base b is a point set consisting of b^m points in $[0,1)^d$ such that every elementary interval of the form

$$\prod_{q=1}^{d} \left[\frac{a_j}{b^{h_j}}, \frac{a_j + 1}{b^{h_j}} \right)$$

with each $h_j \geq 0$, $0 \leq a_j < b^{h_j}$ and $h_1 + \ldots + h_d = m - t$, contains exactly b^t points.

Example: $(0, 4, 2)$-net in base $b = 2$ (Hammersley points).

Discrete least squares with deterministic points

Consider any (t, m, d)-net in base $b \geq 2$ with quality parameter $t \geq 0$.

Theorem (M., Nobile, J.Complexity 2015)

In any dimension d, with the uniform density and with anisotropic tensor product spaces $\mathbb{P}_\Lambda$, if

$$1 > \delta > b^t (b+3)^{d-2} \left(1 + \frac{b-1}{b+3} \frac{\ln M}{\ln b} \right)^{d-1} \mathcal{O}\left(d^2\right) \frac{(\#\Lambda)^2}{M}$$

then it holds that

$$cond(G) \leq \frac{1+\delta}{1-\delta},$$

$$\|\phi - \Pi_\Lambda^M \phi\|_{L^2_\rho} \leq \left(1 + \sqrt{\frac{1}{1-\delta}} \right) \inf_{v \in \mathbb{P}_\Lambda} \|\phi - v\|_{L^\infty}.$$

Similar theorem also for (t, d)-sequences (M.,Nobile, J.Complexity 2015).

Discrete least squares with deterministic points

Three main ingredients in our proof:

1) we prove a variant of the standard Koksma-Hlawka inequality starting from the Hlawka-Zaremba's identity:

Lemma (M., Nobile, J.Complexity 2015)

$$\left| \|f\|_{L^2_\rho}^2 - \|f\|_M^2 \right| \leq \sum_{\emptyset \neq U \subseteq \{1,\dots,d\}} D^{*,U} \sum_{T \subseteq U} \left\| \frac{\partial^{|T|}}{\partial y^T} f(y^U, 1) \right\|_{L^2([0,1]^{|U|})} \left\| \frac{\partial^{|U|-|T|}}{\partial y^{U \setminus T}} f(y^T, 1) \right\|_{L^2([0,1]^{|U|})}.$$

2) Markov-type and Nikolskii-type multivariate inequalities for polynomials associated with downward closed multi-index sets (M., JAT 2015).

3) upper bounds for the star-discrepancy of (t, m, d)-nets and (t, d)-sequences (e.g. Faure-Kritzer, Monatsh. Math. 2013).

Conclusions (theoretical analysis)

RANDOM POINTS: analysis w.r.t. M, d, Λ, ρ, smoothness ϕ:

- in any dimension d, proven stability and accuracy provided that
  - $M/\ln M \geq C_1(\dim(\mathbb{P}_\Lambda))^{\frac{\ln 3}{\ln 2}}$ with Chebyshev density,
  - $M/\ln M \geq C_2(\dim(\mathbb{P}_\Lambda))^2$ with uniform density,
  - $M/\ln M \geq C_3(\dim(\mathbb{P}_\Lambda))^{2\max\{\alpha,\beta\}+2}$ with $\mathrm{beta}(\alpha+1,\beta+1)$, $\alpha,\beta \geq 0$,

  with the constants C_1, C_2, C_3 being independent of d.

DETERMINISTIC POINTS: analysis w.r.t. M, d, Λ, smoothness ϕ:

- in any dimension d, proven stability and accuracy provided that
  - $M \geq \widehat{C}_1(d)(\dim(\mathbb{P}_\Lambda))^2$ with Chebyshev density and any Λ (Zhou et al.),
  - $M/(1+f\ln M)^{d-1} \geq \widehat{C}_2(d)(\dim(\mathbb{P}_\Lambda))^2$ with uniform density and anisotropic tensor product,
  - $M/(1+f\ln M)^{d-1} \geq \widehat{C}_3(d)(\dim(\mathbb{P}_\Lambda))^\gamma,\ 2 \leq \gamma \leq 4$ with uniform density and any Λ downward closed,

  with the constants $\widehat{C}_1$, $\widehat{C}_2$, $\widehat{C}_3$ being dependent on d, and on the parameters of the (t,m,d)-net or (t,d)-sequence.

Conclusions (experience from numerics)

- In high dimensions and with smooth functions, with both random and deterministic points, it seems to be enough

$$M \propto \dim(\mathbb{P}_\Lambda)$$

  to achieve the optimal convergence rate up to a threshold. A lot of numerical evidence, but no formal proof yet.
- Deterministic points CAN outperform random points in low dimensions. What about high dimensions?
- Discrete least squares is a well-promising approximation tool for multivariate aleatory functions and PDEs with stochastic data.

Optimized sets, case of down.closed sets, $d \in \mathbb{N}$

$$\mathcal{M}_n^d := \{\Lambda \subset \mathbb{N}_0^d \ : \ \Lambda \text{ is downward closed and } \#(\Lambda) = n\},$$

$$\Lambda^{opt} := \operatorname*{argmin}_{\Lambda \in \mathcal{M}_n^d} \min_{v \in \mathbb{P}_\Lambda} \|u - v\|_{L^2_\rho} = \operatorname*{argmin}_{\Lambda \in \mathcal{M}_n^d} \sum_{\nu \notin \Lambda} |u_\nu|^2, \quad u_n := \Pi_{\Lambda^{opt}} u.$$

$$\Lambda_M^{opt} := \operatorname*{argmin}_{\Lambda \in \mathcal{M}_n^d} \min_{v \in \mathbb{P}_\Lambda} \|u - v\|_M, \quad w_n := \Pi^M_{\Lambda_M^{opt}} u.$$

Theorem (Cohen-M.-Nobile 201?)

Consider a function u defined on Γ in arbitrary dimension d and let $\gamma > 0$. For any $n \geq 2$, under condition

$$\frac{M}{\ln M} \geq \left(1 + \gamma + \frac{(2n-1)\ln(d(2n-1))}{\ln M}\right) \frac{K(2n-1)}{\beta_{1/2}},$$

it holds that

$$\Pr\left(\|u - w_n\|_{L^2_\rho} \leq (1 + 2\sqrt{2}) \min_{\Lambda \in \mathcal{M}_n^d} \min_{v \in \mathbb{P}_\Lambda} \|u - v\|_{L^\infty(\Gamma)} \right) \geq 1 - 2M^{-\gamma},$$

$$\mathbb{E}(\|u - T_\tau(w_n)\|^2_{L^2_\rho}) \leq 8\sqrt{2}\|u - u_n\|^2_{L^2_\rho} + 8\tau^2 M^{-\gamma}.$$

Optimized sets, case of anchored sets, "$d = \infty$"

Def. Λ anchored: (Λ downward closed) $\wedge$ ($e_j \in \Lambda \implies e_k \in \Lambda, \forall k \leq j$).

$$\mathcal{A}_n := \{\Lambda \subset \mathbb{N}_0^{\mathbb{N}} \ : \ \Lambda \text{ is anchored and } \#(\Lambda) = n\}.$$

$$\tilde{\Lambda}^{opt} := \underset{\Lambda \in \mathcal{A}_n}{\operatorname{argmin}} \min_{v \in \mathbb{P}_\Lambda} \|u - v\|_{L^2_\rho}, \quad \tilde{u}_n := \Pi_{\tilde{\Lambda}^{opt}} u.$$

$$\tilde{\Lambda}^{opt}_M := \underset{\Lambda \in \mathcal{A}_n}{\operatorname{argmin}} \min_{v \in \mathbb{P}_\Lambda} \|u - v\|_M, \quad \tilde{w}_n := \Pi^M_{\tilde{\Lambda}^{opt}_M} u.$$

Theorem (Cohen-M.-Nobile 201?)

Consider a function u defined on $\Gamma = [-1,1]^{\mathbb{N}}$ and let $\gamma > 0$. For any $n \geq 2$, under condition

$$\frac{M}{\ln M} \geq \left(1 + \gamma + \frac{(2n-1)\ln(2n-1)}{\ln M}\right) \frac{K(2n-1)}{\beta_{1/2}},$$

it holds that

$$\Pr\left(\|u - \tilde{w}_n\|_{L^2_\rho} \leq (1 + 2\sqrt{2}) \min_{\Lambda \in \mathcal{A}_n} \min_{v \in \mathbb{P}_\Lambda} \|u - v\|_{L^\infty(\Gamma)} \right) \geq 1 - 2M^{-\gamma},$$

$$\mathbb{E}(\|u - T_\tau(\tilde{w}_n)\|^2_{L^2_\rho}) \leq 8\sqrt{2}\|u - \tilde{u}_n\|^2_{L^2_\rho} + 8\tau^2 M^{-\gamma}.$$

Thank you for your attention!

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