Multilevel discrete least squares polynomial apporixmation

Abdul-Lateef Haji-Ali

Mathematical Institute, University of Oxford

Joint work with: F. Nobile (EPFL), R. Tempone, S. Wolfers (KAUST)

August 14, 2017



1. Problem framework

2. Weighted discrete least squares approximation

Multilevel least squares approximation

Application to random elliptic PDEs

5. Conclusions

PDEs with random parameters

Consider a differential problem

$$\mathcal{L}(u; \mathbf{y}) = \mathcal{G} \tag{(*)}$$

depending on a set of random parameters $\mathbf{y} = (y_1, \dots, y_N) \in \Gamma \subset \mathbb{R}^N$ with joint probability measure μ on Γ . We assume that (*) has a unique solution $u(\mathbf{y})$, in some suitable function space V, and we focus on a Quantity of Interest $Q: V \to \mathbb{R}$.

Goal: approximate the whole response function

$$\mathbf{y} \mapsto f(\mathbf{y}) := Q(u(\mathbf{y})) : \Gamma \to \mathbb{R}$$

by multivariate polynomials.

Possibly derive approximated statistics as $\mathbb{E}[f]$, Var[f], etc.

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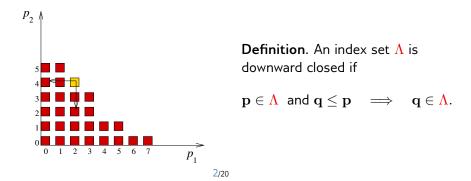
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Polynomial approximation on downward closed sets

Assume $f \in L^2_{\mu}(\Gamma)$. We seek an approximation of f in a finite dimensional polynomial subspace

 $V_{\Lambda} = \operatorname{span} \left\{ \prod_{n=1}^{N} y_n^{p_n}, \text{ with } \mathbf{p} = (p_1, \dots, p_N) \in \Lambda \right\}$ with $\Lambda \subset \mathbb{N}^N$ a downward closed index set.





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Weighted discrete least squares approximation

- 1. Sample independently M points $(\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(M)}) \in \Gamma^M$ from a distribution $\nu \ll \mu$, with density $\rho = \frac{d\nu}{d\mu}$;
- 2. define the weight function $w(\mathbf{y}) = \frac{1}{\rho(\mathbf{y})}$;
- 3. find weighted discrete least squares approximation on V_{Λ}

$$\hat{\Pi}_{\boldsymbol{M}} f = \operatorname*{argmin}_{v \in V_{\Lambda}} \|f - v\|_{\boldsymbol{M}} \quad \text{with} \quad \|g\|_{\boldsymbol{M}}^2 = \frac{1}{M} \sum_{j=1}^{M} w\left(\mathbf{y}^{(j)}\right) g\left(\mathbf{y}^{(j)}\right)^2$$

Here: $\mathbb{E}\left[\|g\|_M^2\right] = \int_{\Gamma} w(\mathbf{y})g(\mathbf{y})^2 \nu(d\mathbf{y}) = \int_{\Gamma} g(\mathbf{y})^2 \mu(d\mathbf{y}) = \|g\|_{L^2_{\mu}}^2.$

Algebraic system: let $\{\phi_j\}_{j=1}^{|\Lambda|}$ be a basis of V_{Λ} , orthonormal w.r.t. μ , and $\hat{\Pi}_M f(\mathbf{y}) = \sum_{j=1}^{|\Lambda|} c_j \phi_j(\mathbf{y})$. Then, $\mathbf{c} = (c_1, \dots, c_{|\Lambda|})^T$ satisfies

$$G\mathbf{c} = \hat{\mathbf{f}}, \qquad G_{i,j} = (\phi_i, \phi_j)_M, \quad \hat{f}_i = (f, \phi_i)_M.$$

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Optimally of discrete least squares approximation

Theorem ([Cohen-Migliorati 2017][Cohen-Davenport-Leviatan 2013])

For arbitrary r > 0 define

$$\kappa_{\boldsymbol{r}} := \frac{1/2(1 - \log 2)}{1 + \boldsymbol{r}} \quad \text{ and } \quad \boldsymbol{K}_{\boldsymbol{\Lambda}, \boldsymbol{w}} := \sup_{\boldsymbol{y} \in \Gamma} \left(w(\boldsymbol{y}) \sum_{j=1}^{|\boldsymbol{\Lambda}|} \phi_i(\boldsymbol{y})^2 \right).$$

$$\begin{split} & \text{If } \frac{M}{\log M} \geq \frac{K_{\Lambda,w}}{\kappa_r}, \text{ then} \\ &= P\left(\|G - I\| \leq \frac{1}{2}\right) > 1 - 2M^{-r}. \\ &= \|f - \hat{\Pi}_M f\|_{L^2_{\mu}} \leq (1 + \sqrt{2}) \inf_{v \in V_{\Lambda}} \|f - v\|_{L^{\infty}_{\sqrt{w}}} \text{ with prob. } > 1 - 2M^{-r}. \\ &= \mathbb{E}\left[\|f - \hat{\Pi}^c_M f\|_{L^2_{\mu}}^2\right] \leq C_M \inf_{v \in V_{\Lambda}} \|f - v\|_{L^2_{\mu}}^2 + 2\|f\|_{L^2_{\mu}}^2 M^{-r} \\ &\quad \text{where } \hat{\Pi}^c_M f = \hat{\Pi}_M f \cdot \mathbf{1}_{\{\|G - I\| \leq \frac{1}{2}\}} \text{ and } C_M = \left(1 + \frac{4\kappa_r}{\log M}\right) \xrightarrow{M \to \infty} 1. \end{split}$$

Sufficient number of points - uniform measure

• Uniform measure: $\mu = \mathcal{U}\left(\prod_{i=1}^{N} \Gamma_{i}\right)$ [Chkifa-Cohen-Migliorati-Nobile-Tempone 2015] When sampling from the same distribution ($\nu = \mu$ and w = 1), then

 $|\Lambda| \le K_{\Lambda,1} \le |\Lambda|^2.$

Hence, (unweighted) discrete least square is stable and optimally convergent under the condition

$$rac{M}{\log M} \geq rac{|\Lambda|^2}{\kappa_r}$$
 (quadratic proportionality).

Sufficient number of points - optimal measure

[Cohen-Migliorati 2017] For arbitrary μ, when sampling from the optimal measure

$$\frac{d\nu^*}{d\mu}(\mathbf{y}) = \rho^*(\mathbf{y}) = \frac{1}{|\Lambda|} \sum_{j=1}^{|\Lambda|} \phi_j(\mathbf{y})^2 \quad \Longrightarrow \quad K_{\Lambda, w^*} = |\Lambda|.$$

Hence, weighted discrete least squares stable and optimal with

$$rac{M}{\log M} \geq rac{|\Lambda|}{\kappa_r}$$
 (linear proportionality).

 Sampling algorithms from the optimal distribution are available (marginalization [Cohen-Migliorati 2017], acceptance rejection

[H.-Nobile-Tempone-Wolfers, 2017])

However, the optimal distribution depends on $\Lambda.$ Not good for adaptive algorithms

Sufficient number of points - Chebyshev measure

Alternatively, for uniform measure μ (or more generally a product measure $\mu = \bigotimes_{j=1}^{N} \mu_j$, with μ_j doubling measure, i.e. $\mu_j(2I) = L\mu_j(I)$) one can sample from the arcsin (Chebyshev) distribution.

$$K_{\Lambda,w} \leq C^N |\Lambda|, \qquad \frac{M}{\log M} \geq \frac{C^N}{\kappa_r} |\Lambda|.$$

Still linear scaling but with a constant exponentially dependent on ${\cal N}.$

Advantage: the sampling measure does not depend on $\Lambda.$ Good for adaptivity.



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In practice $f(\mathbf{y})=Q(u(\mathbf{y}))$ can not be evaluated exactly as it requires the solution of a differential equation.

• We introduce a sequence of approximations f_{n_ℓ} , $n_\ell \in \mathbb{N}$ with increasing cost, s.t.

$$\lim_{\ell \to \infty} \|f - f_{\boldsymbol{n_\ell}}\|_{L^2_{\mu}} = 0,$$

(or possibly a stronger norm)

Similarly, we introduce a sequence of nested downward closed sets

$$\Lambda_{m_0} \subset \Lambda_{m_1} \subset \ldots \subset \Lambda_{m_k} \subset \ldots$$

such that

$$\lim_{k \to \infty} \inf_{v \in V_{\Lambda_{m_k}}} \|f - v\|_{L^2_{\mu}} = 0.$$

Correspondingly, for each Λ_{m_k} we introduce a weighted discrete least squares projector $\hat{\Pi}_{M_k}$ using $\frac{M_k}{\log M_k} = O(|\Lambda_{m_k}|)$ random points. 8/20

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$$S_L f = \sum_{k+\ell \le L} (\hat{\Pi}_{M_k} - \hat{\Pi}_{M_{k-1}}) (f_{n_\ell} - f_{n_{\ell-1}})$$
$$= \sum_{\ell=0}^L \hat{\Pi}_{M_{L-\ell}} (f_{n_\ell} - f_{n_{\ell-1}}).$$

- In the multilevel formula one might consider more general index sets $(k, \ell) \in \mathcal{I} \subset \mathbb{R}^2$. However, one can always recast to $k + \ell \leq L$ by properly choosing $\{n_\ell\}$ and $\{m_k\}$.
- Question: How to properly choose $\{n_{\ell}\}$ and $\{m_k\}$?
- Issue: Since the least squares projection is random, we have to ensure that it is stable and optimally convergent on all levels. (Need union bound on failure probabilities)

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- For the Multilevel algorithm to be effective, we have to rely on certain "mixed regularity".
- Let $(F, \|\cdot\|_F) \hookrightarrow (L^2_{\mu}, \|\cdot\|_{L^2_{\mu}})$ be a normed vector space of "smooth" functions (e.g. Hölder / Sobolev / analytic regularity).

Assumption 1 (regularity): $f, f_{n_{\ell}} \in F$ for all $\ell \in \mathbb{N}$

Assumption 2 (PDE discretization): the sequence { f_{n_ℓ} } is s.t.

$$\|f - f_{n_{\ell}}\|_{L^{2}_{\mu}} \lesssim n_{\ell}^{-\beta_{w}}, \qquad \|f - f_{n_{\ell}}\|_{F} \lesssim n_{\ell}^{-\beta_{s}}$$

and, for a single $\mathbf{y} \in \Gamma$, the cost of computing $f_{n_{\ell}}(\mathbf{y})$ is
 $\operatorname{Work}(f_{n_{\ell}}) \lesssim n_{\ell}^{\gamma}.$

• Assumption 3 (polynomial approximability): the sequence $\{\Lambda_{m_k}\}$ is s.t.

$$\dim \left(V_{\Lambda_{m_k}} \right) = |\Lambda_{m_k}| \lesssim m_k^{\sigma},$$
$$\inf_{v \in V_{\Lambda_{m_k}}} \|f - v\|_{L^{\infty}_{\sqrt{w}}} \lesssim m_k^{-\alpha_p} \|f\|_F, \quad \forall f \in F,$$
Alternatively
$$\inf_{v \in V_{\Lambda_{m_k}}} \|f - v\|_{L^2_{\mu}} \lesssim m_k^{-\alpha_e} \|f\|_F, \quad \forall f \in F).$$

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Tuning the ML least squares algorithm

We now choose

$$\begin{split} n_{\ell} &= C \exp\left(\frac{\ell}{\gamma + \beta_s}\right), \quad \ell = 0, \dots, L \quad \text{(space discr.)} \\ m_k &= C \exp\left(\frac{k}{\sigma + \alpha_p}\right), \quad k = 0, \dots, L \quad \text{(Polynomial approx.)} \\ \frac{m_k^{\sigma}}{\kappa_L} &\leq \frac{M_k}{\log M_k} \leq \frac{2m_k^{\sigma}}{\kappa_L}, \quad k = 0, \dots, L \quad \text{(sample size with } r = L\text{)} \end{split}$$

By taking r=L we guarantee that

$$P\left(\exists k: \|G_k - I\| > \frac{1}{2}\right) \leq \sum_{k=0}^{L} P\left(\|G_k - I\| > \frac{1}{2}\right) \lesssim L^{-L}.$$

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Complexity result

Theorem ([H.-Nobile-Tempone-Wolfers 2017])

Given $\epsilon>0$ and $\beta_s=\beta_w$, we can choose $L\in\mathbb{N}$ such that

$$\|f - S_L f\|_{L^2_{\mu}} \le \epsilon, \quad \text{with prob.} \ge 1 - C\epsilon^{\log|\log\epsilon|},$$
$$\operatorname{Work}(S_L f) \lesssim \epsilon^{-\lambda} |\log\epsilon|^t \log|\log\epsilon|,$$

with

$$\begin{split} \lambda &= \max \left(\sigma / \alpha_p, \gamma / \beta_s \right), \\ t &= \begin{cases} 2 & \text{if } \gamma / \beta_s < \sigma / \alpha_p, \\ 3 + \sigma / \alpha_p & \text{if } \gamma / \beta_s = \sigma / \alpha_p, \\ 1 & \text{if } \gamma / \beta_s > \sigma / \alpha_p. \end{cases} \end{split}$$

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Analogous result holds in expectation with $lpha_p$ replaced by $lpha_e$

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Improved complexity in the case $\gamma/\beta_s > \sigma/\alpha$

In the case $\gamma/\beta_s > \sigma/\alpha$ and $\beta_w > \beta_s$ the complexity can be improved by taking

$$m_k = C \exp\left(\frac{k}{\sigma + \alpha_p} + \frac{L(\beta_w - \beta_s)}{\alpha(\gamma + \beta_s)}\right).$$

In this case the complexity result becomes

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$$\lambda = \frac{\gamma}{\beta_w} + \left(1 - \frac{\beta_s}{\beta_w}\right) \frac{\sigma}{\alpha_p}$$

which always improves the single level rate $\lambda_{SL} = \frac{\gamma}{\beta_w} + \frac{\sigma}{\alpha_p}$.

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Application to random elliptic PDEs

Consider

$$\begin{cases} -\operatorname{div}(\boldsymbol{a}(\mathbf{y})\nabla u(\mathbf{y})) = g, & \text{in } D \subset \mathbb{R}^d\\ u(\mathbf{y}) = 0, & \text{on } \partial D \end{cases}$$

with $\mathbf{y} \in \Gamma = [-1, 1]^N$ and Q linear bounded functional in $L^2(D)$ (e.g. $Q(u) = \int_D u$).

Goal: approximate $f(\mathbf{y}) = Q(u(\mathbf{y}))$.

Assumptions:

- $0 < a_{min} \le a(\mathbf{x}, \mathbf{y}) \le a_{max}, \quad \forall (\mathbf{x}, \mathbf{y}) \in D \times \Gamma.$
- g and D sufficiently smooth.

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- $0 < a_{min} \le a(\mathbf{x}, \mathbf{y}) \le a_{max}, \quad \forall (\mathbf{x}, \mathbf{y}) \in D \times \Gamma.$
- g and D sufficiently smooth.

Application to random elliptic PDEs

Consider

$$\begin{cases} -\operatorname{div}(\boldsymbol{a}(\mathbf{y})\nabla u(\mathbf{y})) = g, & \text{in } D \subset \mathbb{R}^d\\ u(\mathbf{y}) = 0, & \text{on } \partial D \end{cases}$$

with $\mathbf{y} \in \Gamma = [-1, 1]^N$ and Q linear bounded functional in $L^2(D)$ (e.g. $Q(u) = \int_D u$).

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Application to random elliptic PDEs

Proposition

Let u_n be a finite element approximation of order $r \ge 1$ with maximal element diameter $h = n^{-1}$ and $f_n(\mathbf{y}) = Q(u_n(\mathbf{y}))$.

• If $a \in C^r(D \times \Gamma)$, then

$$||f - f_n||_{L^2_{\mu}(\Gamma)} \lesssim h^{r+1}, \qquad ||f - f_n||_{C^{r-1}(\Gamma)} \lesssim h^2.$$

• If $a \in C^{r,s}(D \times \Gamma) = \{v : D \times \Gamma \to \mathbb{R} : \|\partial_x^{\mathbf{r}} \partial_y^{\mathbf{s}} v\|_{C^0(D \times \Gamma)} < \infty, \forall |\mathbf{r}|_1 \le r, |\mathbf{s}|_1 \le s \}$, then

$$||f - f_n||_{C^p(\Gamma)} \lesssim h^{r+1}, \qquad \forall p = 0, \dots, s.$$

ML least squares complexity – mixed regularity

Consider the coefficient

$$a(\mathbf{x}, \mathbf{y}) = 1 + \|\mathbf{x}\|_{2}^{r} + \|\mathbf{y}\|_{2}^{s} \in C^{r-1,1}(D) \otimes C^{s-1,1}(\Gamma).$$

• smoother space: $F = C^{s-1,1}(\Gamma)$;

- spatial approximation: continuous finite elements of degree r,
 - ► error: $||f f_n||_{L^2_{\mu}} = O(n^{-(r+1)}) = ||f f_n||_{C^{s-1,1}} \implies \beta_w = \beta_s = r+1;$

► cost: $Work(f_n) = n^d$ with optimal solver $\implies \gamma = d$;

Polynomial approximation: $V_{\Lambda_m} = \mathbb{P}_m$ = polynomial space of total degree m,

► error:
$$||f - \prod_{\mathbb{P}_m} f||_{L^{\infty}} = O(m^{-s}), \implies \alpha_p = s;$$

► cost: dim $(V_{\bullet}) = \binom{m+N}{2} \le m^N \implies \sigma = N$

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$$(V_{\Lambda_m}) = \binom{m+N}{N} \lesssim m^N$$
, $\implies \sigma = N$.

ML least squares complexity – mixed regularity

Complexity of single level method

Work_{SL} =
$$\mathcal{O}\left(\epsilon^{-\frac{d}{r+1}-\frac{N}{s}}\log\epsilon^{-1}\right)$$
.

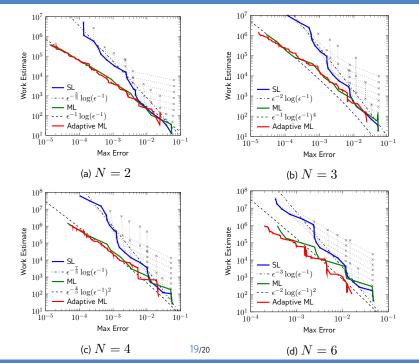
Complexity of multilevel method

Work_{ML} =
$$\mathcal{O}\left(\epsilon^{-\max\left\{\frac{d}{r+1},\frac{N}{s}\right\}}\left(\log\epsilon^{-1}\right)^{t}\right)$$
,

with

$$t = \begin{cases} 1, & \text{if } \frac{d}{r+1} > \frac{N}{s}, \\ 3 + \frac{d}{r+1}, & \text{if } \frac{d}{r+1} = \frac{N}{s}, \\ 2, & \text{if } \frac{d}{r+1} < \frac{N}{s}. \end{cases}$$

In our experiment: d = 2, r = 1, s = 3 and N = 2, 3, 4, 6.





1. Problem framework

2. Weighted discrete least squares approximation

Multilevel least squares approximation

4. Application to random elliptic PDEs

- We have derived a multilevel discrete least squares method for polynomial approximation of an output quantity of interest of a random PDE.
- The method uses the classical "Combination technique" and sparsifies sequences of polynomial approximations, obtained by weighted discrete least squares, and sequences of spatial discretizations of the underlying PDE.
- In particular, we have proposed a way to select the number of sample points on each level to guarantee the overall stability and accuracy of the ML formula with high probability.
- Complexity analysis carries over to infinite dimensional problems (different choice of polynomial spaces).
- We are currently working on adaptive algorithms for infinite dimensional problems.

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Thank you for your attention.

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Sketch of the proof

Bound on M_k : use that $\sqrt{M_k} \le \frac{M_k}{\log M_k} \le \frac{2m_k^{\sigma}}{\kappa_L}$ and $\kappa_L \approx 1/(L+1)$

$$M_k \le \frac{2}{\kappa_L} m_k^{\sigma} \log M_k \lesssim (L+1) e^{\frac{k\sigma}{\sigma+\alpha_p}}$$
$$\lesssim (L+1) \log(L+1) e^{\frac{k\sigma}{\sigma+\alpha_p}} (k+1)$$

Bound on total work:

$$\operatorname{Work}(S_L f) \lesssim \sum_{\ell=0}^{L} M_{L-\ell} n_{\ell}^{\gamma}$$
$$\lesssim (L+1) \log(L+1) e^{\frac{L\sigma}{\sigma-\alpha_p}} \sum_{\ell=0}^{L} \exp\left\{-l\left(\frac{\sigma}{\sigma-\alpha_p} - \frac{\gamma}{\gamma+\beta_s}\right)\right\} (L-\ell+1)$$

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Sketch of the proof

Bound on the error in probability:

$$\begin{split} \|f - S_L f\|_{L^2_{\mu}} &= \|f - f_L + \sum_{\ell=0}^{L} (Id - \hat{\Pi}_{M_{L-\ell}})(f_\ell - f_{\ell-1})\|_{L^2_{\mu}} \\ &\leq \|f - f_L\|_{L^2_{\mu}} + \sum_{\ell=0}^{L} \|Id - \hat{\Pi}_{M_{L-\ell}}\|_{F \to L^2_{\mu}} \|f_\ell - f_{\ell-1}\|_F \\ &\lesssim e^{-\frac{L\beta_w}{\gamma + \beta_s}} + e^{-\frac{L\alpha}{\sigma + \alpha}} \sum_{\ell=0}^{L} \exp\left\{\ell\left(\frac{\alpha}{\sigma + \alpha_p} - \frac{\beta_s}{\gamma + \beta_s}\right)\right\} \end{split}$$

Again split the three cases $\gamma/\beta_s <, =, > \sigma/\alpha_p$ and notice that the first term $e^{-\frac{L\beta_w}{\gamma+\beta_s}}$ is always negligible as $\beta_w > \beta_s$.

