Autoencoders and Reduced Bases

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Nonlinear Approximation for High-Dimensional Problems

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in Honor of Albert Cohen

Deep Neural Networks (DNN) Autoencoders

Analyze a compact set K in a metric space X by transforming its elements to a low dimensional space Y and keeping the essential information about them.

- *encoder* $E : X \to Y$ and *decoder* $D : Y \to X$
- for any element $x \in K$ we want $\mathrm{dist}_X\big(x, D(E(x))\big)$ to be small
- given a measure μ on K consider $\int_K \mathrm{dist}_X\big(x, D(E(x))\big) d\mu$
- other measures of closeness $\sup_{x\in K} \mathrm{dist}_X\big(x, D(E(x))\big)$
  or if X is a normed space, $\int_K \|x - D(E(x))\|_X^2 d\mu$

Autoencoders are DNNs that have an encoder part E and a decoder part D.

- X can be an infinite dimensional or a very high dimensional space
- consider a discretization of X to $\mathbb{R}^N$ $\rightsquigarrow$ use X for it, e.g. $X = \ell_2(\mathbb{R}^N)$
- usually $Y = \ell_2(\mathbb{R}^d)$ with $N \gg d$ but we can consider other norms/metrics
- typical *loss function* $L(E, D) = \sum_{j=1}^K \|x_j - D(E(x_j))\|_X^2$

Autoencoders Setup

- the objective is to consider $K \subset X$ via random sampling of its elements and attempt to describe it in terms of the elements of a *latent* space Y
- the *autoencoder* $A(x) := D(E(x))$ and aiming at $x \approx A(x)$
- the encoder $E : X \to Y$ depends on several parameters $\mathcal{E}$: $E(x) = E(\mathcal{E}; x)$ it is composed of several layers $E(x) = E_{\ell_E}(...(E_2(E_1(x)))...)$:

  $x^{[1]} = E_1(\mathcal{E}_1; x)$, $x^{[2]} = E_2(\mathcal{E}_2; x^{[1]})$, ... , $y = x^{[\ell_E]} = E_{\ell_E}(\mathcal{E}_{\ell_E}; x^{[\ell_E - 1]})$

  with parameter set $\mathcal{E} = \cup_{j=1}^{\ell_E} \mathcal{E}_j$
- the decoder $D : Y \to X$ depends on the parameters $\mathcal{D}$: $D(y) = D(\mathcal{D}; y)$ it is composed of several layers $D(y) = D_{\ell_D}(...(D_2(D_1(y)))...)$:

  $y^{[1]} = D_1(\mathcal{D}_1; y)$, $y^{[2]} = D_2(\mathcal{D}_2; y^{[1]})$, ... , $\tilde{x} = y^{[\ell_D]} = D_{\ell_D}(\mathcal{D}_{\ell_D}; y^{[\ell_D - 1]})$

  with parameter set $\mathcal{D} = \cup_{j=1}^{\ell_D} \mathcal{D}_j$

Autoencoders Setup

- for $x \in K$ set $y = E(x)$ and $\tilde{x} = D(y) = A(x)$; data points $x_j \in K$, $j \in J$
- the loss function can be $L(E,D) = \frac{1}{\#J} \sum_{j \in J} \|x_j - A(x_j)\|_X^2$
  or $L(E,D) = \frac{1}{\#J} \sum_{j \in J} \|x_j - A(x_j)\|_X^2 + \frac{1}{\#J} \sum_{j \in J} \|E(x_j)\|_Y^2$
- the setup can use a distance instead of a norm and any ℓ_p averaging, $1 \le p \le \infty$, instead of the averaged ℓ_2-norms
- the main issue is to define the sets $\mathfrak{E}$ and $\mathfrak{D}$ over which the search for (the parameter sets $\mathcal{E}$ and $\mathcal{D}$ of) $E \in \mathfrak{E}$ and $D \in \mathfrak{D}$ is performed
- note that the performance of the autoencoder depends on

$$\inf_{D \in \mathcal{D}} \sup_{x \in K} \inf_{y \in Y} \|x - D(y)\|_X$$

Reduced Basis

Find a basis of a low-dimensional linear space that approximates well a compact set K of interest – often the set of solutions of a parametric PDE

[Maday, Y., Patera, A.T., Turinici, G.: A priori convergence theory for reduced-basis approximations of single-parametric elliptic partial differential equations. J. Sci. Comput. 17, 437–446 (2002)]

Use a greedy algorithm to find such a basis:

- [Buffa, A., Maday, Y., Patera, A.T., Prud'homme, C., Turinici, G.: A Priori convergence of the greedy algorithm for the parameterized reduced basis. Modél. Math. Anal. Numér. 46, 595–603 (2012)]
- [Binev, P., Cohen, A., Dahmen, W., DeVore, R., Petrova, G., Wojtaszczyk, P.: Convergence rates for greedy algorithms in reduced bases Methods. SIAM J. Math. Anal. 43, 1457–1472 (2011)]
- [DeVore, R., Petrova, G., Wojtaszczyk, P.: Greedy algorithms for reduced bases in Banach spaces, Constructive Approximation 37, 455–466 (2013)]

Building of a Reduced Basis by a *Random* Greedy Selection

- x_j – independent and identically distributed (iid) random drawings from K
- choose $u_1 := x_m$ for $m = \text{argmax}_{j \in J} \|x_j\|_X$
- choose $u_{k+1} := x_m$ for $m = \text{argmax}_{j \in J} \min_{u \in \text{span}\{u_1, \dots u_k\}} \|x_j - u\|_X$
- it is convenient to orthonormalize the basis $u_1, u_2, \dots, u_n$
- to use the theorems about the greedy selection of the reduced basis we need that for $U_k := \text{span}\{u_1, \dots u_k\}$

$$\min_{u \in U_k} \|u_{k+1} - u\|_X \geq \gamma \sup_{x \in K'} \min_{u \in U_k} \|x - u\|_X$$

for some fixed $\gamma \in (0, 1]$ with high probability on $x \in K$

meaning that the set $K' \subset K$ has measure $\mu(K') \geq 1 - \delta$ for some very small $\delta > 0$, where μ is the probability measure of K

Reduced Basis Greedy Selection using Random Training Sets

[Cohen, A., Dahmen, W., DeVore, R., Nichols, J.: Reduced Basis Greedy Selection Using Random Training Sets, ESAIM: M2AN 54, 1509–1524 (2020)]

- fine discretization by a random training set of size polynomial in ε^{-1} to obtain a final approximation error ε with high probability
- Σ_m – union of polynomial spaces with downward closed bases of size m
- $K \subset X$ is a compact set of mappings $v \to x(v)$ for parameter sets $v \in V$
- approximation class $\mathcal{A}^r := \{x \in X : \inf\limits_{P \in \Sigma_m} \sup\limits_{v \in V} \|x(v) - P(v)\|_X < Cm^{-r}\}$

Theorem. Let $K \subset \mathcal{A}^r$ for $r > 2$ and $C \leq M_0$ in the definition be bounded. Then with probability greater than $1 - \eta$ the weak greedy algorithm produces a reduced basis space U_n such that $\operatorname{dist}(K, U_n) \leq \varepsilon$ and if for some $s > 0$ the Kolmogorov width $d_n(K)$ behaves as n^{-s}, then $n = n(\varepsilon) \leq C_0 e^{-(\frac{1}{s} + \frac{3}{s(r-2)})}$ and the error bound evaluations are $N(\varepsilon) \leq C_0 e^{-\frac{2s+r+1}{s(r-2)}}(|\log \varepsilon| + |\log \eta|)$.

Probability Inequalities

We assume minimal requirements about the set K and the random selection $\{x_j\}_{j\in J}$ that include the assumption that can estimate well the first three moments $\mathbf{E}\mathcal{Z}$, $\mathbf{E}\mathcal{Z}^2$, and $\mathbf{E}\mathcal{Z}^3$ of random variables $\mathcal{Z}$ under consideration

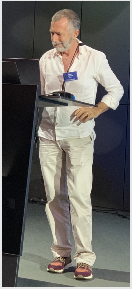
$\mathcal{Z}$ is the random variable representing the approximation error on the k-th step of the greedy algorithm. We estimate it by the random sampling $\{x_j\}_{j\in J}$ from K. The estimation z_k should be bounded by $z_k \geq \gamma M_k$ with $\gamma > 0$ large enough, where M_k is the actual maximum of such an error over all elements of K

- Chebyshev inequality: $\mathbf{Prob}\Big(\mathcal{Z} - \mathbf{E}\mathcal{Z} \geq \alpha\big(\mathbf{E}\mathcal{Z}^2 - [\mathbf{E}\mathcal{Z}]^2\big)\Big) \leq \frac{1}{\alpha^2}$
- set $\alpha = \frac{M}{\mathbf{E}\mathcal{Z}^2 - [\mathbf{E}\mathcal{Z}]^2}$, where M is the predicted maximal value of $\mathcal{Z}$ on K, so we have to increase M and by this decrease γ to make $\delta = \frac{1}{\alpha^2}$ very small
- the above estimate does not depend on the number of drawings $\#J$ we have
- we need inverted Chebyshev inequality to have such an estimate

Estimate of the Maximum of the Errors

- consider the realizations z_j of $\mathcal{Z}$ representing the errors at the k-th step of the greedy algorithm
- $\mathbf{Prob}(\max_{j \in J} z_j < \gamma M_k) = \Big(\mathbf{Prob}(z_j < \gamma M_k)\Big)^{\# J}$
  $= \Big(1 - \mathbf{Prob}(z_j \geq \gamma M_k)\Big)^{\# J}$
- [Rohatgi, V.K., Szekely, G.J.: An Inverse Markov-Chebyshev Inequality, Periodica Polytechnica Ser. Civil Eng. 36, 455–458 (1992)]
- estimates of $\mathbf{Prob}(\mathcal{Z} > a)$ from below using the first three moments of $\mathcal{Z}$ for example, $\mathbf{Prob}(\mathcal{Z} > a) \geq -2\frac{\mathbf{E}\mathcal{Z}}{a} + \frac{11}{4}\frac{\mathbf{E}\mathcal{Z}^2}{a^2} - \frac{3}{4}\frac{\mathbf{E}\mathcal{Z}^3}{a^3}$
- work in progress with Edsel Pena, Henry Simmons, and Josh Moorehead

Happy Birthday Albert!



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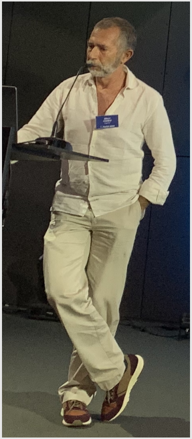

Best wishes and good luck!