

Random Neural Network Approximation of Dynamic Barron Functions

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based on joint work with Lyudmila Grigoryeva and Juan-Pablo Ortega

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Overview

- Reservoir computing & echo state networks: highly efficient at learning dynamical / chaotic systems (see, e.g., Jaeger & Haas [JH04], Pathak, Hunt, Girvan, Lu & Ott [PHG⁺18], ...).
- **Learning theoretical foundations?**
 - Universality:
 - Grigoryeva & Ortega, *Neural Netw.* (2018) [GO18]
 - G. & Ortega, *IEEE TNNLS* (2020) [GO20]
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 - Generalization error: G., Grigoryeva & Ortega *JMLR* (2020) [GGO20]
 - Approximation error: G., Grigoryeva & Ortega *Ann. Appl. Probab.* (2022+) [GGO22]
 - RC systems via random projection: Cuchiero et al. *IEEE TNNLS* (2021) [CGG⁺21]
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- Quantitative bounds: for sufficiently smooth functionals.
- Goal: **full learning error bounds for inherently infinite-dimensional**, not necessarily smooth functionals.

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Neural network approximation

Let us look at **neural network approximation** in the much further developed **static case**:

Neural networks are able to overcome the curse of dimensionality for classes of

- compositional functions (built from lower-dimensional functions),
- solutions to certain PDEs,
- Barron functions / functions with dimension-dependent regularity.
 - Originally proposed by Barron [Bar92], [Bar93].
 - Extended to the larger class of “generalized Barron functions” in E et al. [EW20], [EMWW20], [EMW19].
 - Goal: **dynamic analogue**
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 - Approximation and learning bounds.

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Recurrent generalized Barron functionals

- Let $D_d \subset \mathbb{R}^d$ bounded, $\mathcal{I}_d \subset (D_d)^{\mathbb{Z}_-}$,
- $\sigma_1, \sigma_2: \mathbb{R} \rightarrow \mathbb{R}$ activations (applied componentwise),
- $p \in [1, \infty]$, q such that $\frac{1}{p} + \frac{1}{q} = 1$.

Definition

$H: \mathcal{I}_d \rightarrow \mathbb{R}$ is called **recurrent generalized Barron functional**, if there exist

- a probability measure μ on $\mathbb{R} \times \ell^p \times \mathbb{R}^d \times \mathbb{R}$ with finite expectation,
- $B \in \ell^q$ and linear maps $A: \ell^q \rightarrow \ell^q$, $C: \mathbb{R}^d \rightarrow \ell^q$

such that for each $\mathbf{z} \in \mathcal{I}_d$ the system

$$\mathbf{x}_t = \sigma_1(A\mathbf{x}_{t-1} + C\mathbf{z}_t + B), \quad t \in \mathbb{Z}_-,$$

admits a unique solution $(\mathbf{x}_t)_{t \in \mathbb{Z}_-}$ with $\mathbf{x}_t = \mathbf{x}_t(\mathbf{z}) \in \ell^q$ and

$$H(\mathbf{z}) = \int_{\mathbb{R} \times \ell^p \times \mathbb{R}^d \times \mathbb{R}} w \sigma_2(\mathbf{a} \cdot \mathbf{x}_{-1}(\mathbf{z}) + \mathbf{c} \cdot \mathbf{z}_0 + b) \mu(dw, d\mathbf{a}, d\mathbf{c}, db), \quad \mathbf{z} \in \mathcal{I}_d.$$

Properties

Denote by \mathcal{H} the class of all recurrent generalized Barron functionals. For natural choices of activation functions ($\sigma_1(x) = x$ and either $\sigma_2(x) = \max(x, 0)$ or σ_2 is bounded, continuous and non-constant) we obtain:

- \mathcal{H} is a vector space
- \mathcal{H} contains
 - sufficiently smooth functionals
 - functionals associated to convolutional filters
- $\mathcal{H} \cap L^{\bar{p}}(\mathcal{I}_d, \gamma)$ is dense in $L^{\bar{p}}(\mathcal{I}_d, \gamma)$ for any $\bar{p} \in [1, \infty)$ and any probability measure γ on $\mathcal{I}_d \subset (D_d)^{\mathbb{Z}_-}$.

Key example

Proposition

Suppose $p = 2$. Let \mathcal{Y} be a separable Hilbert space, let $\bar{A}: \mathcal{Y} \rightarrow \mathcal{Y}$, $\bar{C}: \mathbb{R}^d \rightarrow \mathcal{Y}$ be linear and $\bar{B} \in \mathcal{Y}$ and assume that for each $\mathbf{z} \in \mathcal{I}_d$ the system

$$\bar{\mathbf{x}}_t = \bar{A}\bar{\mathbf{x}}_{t-1} + \bar{C}\mathbf{z}_t + \bar{B}, \quad t \in \mathbb{Z}_-, \quad (1)$$

admits a unique solution $(\bar{\mathbf{x}}_t)_{t \in \mathbb{Z}_-} \in \mathcal{Y}^{\mathbb{Z}_-}$. Let $\bar{\mu}$ be a (Borel) probability measure on $\mathbb{R} \times \mathcal{Y} \times \mathbb{R}^d \times \mathbb{R}$ with

$\int_{\mathbb{R} \times \mathcal{Y} \times \mathbb{R}^d \times \mathbb{R}} |w|(\|\mathbf{a}\|_{\mathcal{Y}} + \|\mathbf{c}\| + |b|)\bar{\mu}(dw, d\mathbf{a}, d\mathbf{c}, db) < \infty$ and consider

$$H(\mathbf{z}) = \int_{\mathbb{R} \times \mathcal{Y} \times \mathbb{R}^d \times \mathbb{R}} w \sigma_2(\langle \mathbf{a}, \bar{\mathbf{x}}_{-1}(\mathbf{z}) \rangle_{\mathcal{Y}} + \mathbf{c} \cdot \mathbf{z}_0 + b) \bar{\mu}(dw, d\mathbf{a}, d\mathbf{c}, db), \quad \mathbf{z} \in \mathcal{I}_d. \quad (2)$$

Then $H \in \mathcal{H}$.

Such systems arise, e.g., in quantum reservoir computing.

Learning system

Goal: approximate (unknown) $H \in \mathcal{H}$ using random neural networks:

- Dynamics: captured by a (possibly linear) echo state network mapping an input \mathbf{z} to

$$\mathbf{x}_t^{\text{ESN}} = \sigma_1(\mathbf{A}^{\text{ESN}} \mathbf{x}_{t-1}^{\text{ESN}} + \mathbf{C}^{\text{ESN}} \mathbf{z}_t + \mathbf{B}^{\text{ESN}}), \quad t \in \mathbb{Z}_-, \quad (3)$$

with given (randomly generated) matrices $\mathbf{B}^{\text{ESN}} \in \mathbb{R}^N$, $\mathbf{A}^{\text{ESN}} \in \mathbb{R}^{N \times N}$, $\mathbf{C}^{\text{ESN}} \in \mathbb{R}^{N \times d}$.

- Random feedforward neural network readout: H is approximated by

$$\hat{H}(\mathbf{z}) = \hat{H}_{\mathbf{W}}(\mathbf{z}) = \sum_{i=1}^N W_i \sigma_2(\mathbf{a}^{(i)} \cdot \mathbf{x}_{-1}^{\text{ESN}}(\mathbf{z}) + \mathbf{c}^{(i)} \cdot \mathbf{z}_0 + b_i) \quad (4)$$

with randomly generated coefficients $\mathbf{a}^{(i)}$, $\mathbf{c}^{(i)}$, b_i valued in \mathbb{R}^N , \mathbb{R}^d and \mathbb{R} , respectively.

- Only $\mathbf{W} \in \mathbb{R}^N$ is trainable.

Approximation result

- Let $T = \lceil \frac{N}{d} \rceil$ and suppose \mathbf{A}^{ESN} , \mathbf{C}^{ESN} are generated so that $\|\mathbf{A}^{\text{ESN}}\| < 1$ and K is invertible, with
$$K = \pi_{N \times N}(\mathbf{C}^{\text{ESN}} | \mathbf{A}^{\text{ESN}} \mathbf{C}^{\text{ESN}} | \dots | (\mathbf{A}^{\text{ESN}})^{T-2} \mathbf{C}^{\text{ESN}} | (\mathbf{A}^{\text{ESN}})^{T-1} \mathbf{C}^{\text{ESN}}).$$
- Suppose $H \in \mathcal{H}$ with $\|A\| < 1$, μ has finite second moments.
- Assume that hidden readout weights are sampled from a generic measure ν satisfying an absolute continuity condition w.r.t. μ .

Theorem (Approximation error bound)

Consider the setting above and let $\sigma_1(x) = x$, $p \in (1, \infty)$, $\lambda \in (\|A\|, 1)$. Then there exists f such that \hat{H} with readout $\mathbf{W} = f((w^{(i)}, \mathbf{a}^{(i)}, \mathbf{c}^{(i)}, b_i)_{i=1, \dots, N})$ satisfies for any $\mathbf{z} \in \mathcal{I}_d$

$$\mathbb{E}[|H(\mathbf{z}) - \hat{H}(\mathbf{z})|^2]^{1/2} \leq C_{H, \text{ESN}} [\lambda^{\frac{N}{d}} + \|\mathbf{A}^{\text{ESN}}\|^T + \frac{1}{N^{\frac{1}{2}}}]$$

The constant $C_{H, \text{ESN}}$ is available explicitly.

Approximation result

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The constant $C_{H, \text{ESN}}$ is available explicitly.

- Suppose the dynamic learning part (in particular \mathbf{A}^{ESN} , \mathbf{B}^{ESN} , \mathbf{C}^{ESN}) remains “bounded” in N , i.e.,
 - there exists $\bar{c} > 0$ and $\underline{l}, \bar{l} \in (0, 1)$, $\underline{l} < \bar{l}$ such that for any choice of N the ESN parameters satisfy that
 - K is invertible
 - $\underline{l} < \|\mathbf{A}^{\text{ESN}}\| < \bar{l}$
 - $\|\mathbf{B}^{\text{ESN}}\| \leq \bar{c}$, $\|\mathbf{C}^{\text{ESN}}\| \leq \bar{c}$
 - $\|K^{-1} \text{diag}(\mathbb{1}_d, \mathbb{1}_d \underline{l}^{k-1}, \dots, \underline{l}^{T-1})\| \leq \bar{c}$

\Rightarrow the constant $C_{H, \text{ESN}}$ does not depend on N .

Universality

Let σ_1, σ_2 as before.

Corollary

Let $H: \mathcal{I}_d \rightarrow \mathbb{R}$ be an arbitrary functional and let ν_0 be a given hidden weight distribution with finite first moment.

Then for any $\varepsilon > 0$ and any probability measure γ on $\mathcal{I}_d \subset (D_d)^{\mathbb{Z}^-}$ with $H \in L^2(\mathcal{I}_d, \gamma)$ there exists a probability measure ν with $\mathcal{W}_1(\nu_0, \nu) < \varepsilon$ and a readout \mathbf{W} such that \hat{H} with readout \mathbf{W} and distribution ν for the hidden layer weights satisfies

$$\left(\int_{\mathcal{I}_d} \mathbb{E}[|H(\mathbf{z}) - \hat{H}(\mathbf{z})|^2] \gamma(d\mathbf{z}) \right)^{1/2} < \varepsilon.$$

Special case: static situation

- Let μ_0 be a probability measure on $\mathbb{R} \times \mathbb{R}^d \times \mathbb{R}$ and

$$H(\mathbf{u}) = \int_{\mathbb{R} \times \mathbb{R}^d \times \mathbb{R}} w \sigma_2(\mathbf{c} \cdot \mathbf{u} + b) \mu_0(dw, d\mathbf{c}, db), \quad \mathbf{u} \in D_d \subset \mathbb{R}^d.$$

- $$\hat{H}(\mathbf{u}) = \sum_{i=1}^N W_i \sigma_2(\mathbf{c}^{(i)} \cdot \mathbf{u} + b_i)$$

is used as learning system with randomly generated $\mathbf{c}^{(i)}$, b_i (distribution ν_0) and $\mathbf{W} \in \mathbb{R}^N$ trainable.

Corollary

Let H as above with $\mu_0 \ll \nu_0$. Then there exists \mathbf{W} s. t. for any $\mathbf{u} \in D_d$

$$\mathbb{E}[|H(\mathbf{u}) - \hat{H}(\mathbf{u})|^2]^{\frac{1}{2}} \leq \frac{c}{N^{\frac{1}{2}}} \left\| \frac{d\mu_0}{d\nu_0} \right\|_{\infty}^{\frac{1}{2}} \left(\int w^2 [|\mathbf{c}|^2 + |b|^2 + 1] \mu_0(dw, d\mathbf{c}, db) \right)^{\frac{1}{2}},$$

where $c = (2 \max(2L_{\sigma_2}, |\sigma_2(0)|^2) \max(1, \sup_{\mathbf{v} \in D_d} \|\mathbf{v}\|^2))^{\frac{1}{2}}$.

Learning error bounds

How about learning H from a single trajectory of input/output pairs?

- Observations $(\mathbf{Z}_t, \mathbf{Y}_t)_{t=0, -1, \dots, -n+1}$ are available.
- Let $H \in \mathcal{H}$ be the unknown functional and assume that the input/output relation between the data is given as $H(\mathbf{Z}) = \mathbb{E}[\mathbf{Y}_0 | \mathbf{Z}]$
 - Example: $\mathbf{Y}_t = H(\mathbf{Z}_{t+}) + \varepsilon_t$ for a stationary process $(\varepsilon_t)_{t \in \mathbb{Z}_-}$ independent of \mathbf{Z} and with $\mathbb{E}[\varepsilon_0] = 0$.
- To learn H from the data we solve

$$\hat{\mathbf{W}} = \arg \min_{\mathbf{W}} \frac{1}{n} \sum_{i=0}^{n-1} \|\hat{H}_{\mathbf{W}}(\mathbf{Z}_{-i}^{-n+1}) - \mathbf{Y}_{-i}\|^2 \quad (5)$$

where we denote $\mathbf{Z}_{-i}^{-n+1} = (\dots, 0, 0, \mathbf{Z}_{-n+1}, \dots, \mathbf{Z}_{-i-1}, \mathbf{Z}_{-i})$.

- Data points are not i.i.d., but only weakly dependent.

Theorem

Consider the setting as above, let $R \geq \frac{c}{\sqrt{N}}$, assume \mathbf{Y} is bounded and (\mathbf{Z}, \mathbf{Y}) has a causal Bernoulli shift structure with geometric decay of rate λ_{dep} and $\log(n) < n \log(\lambda_{\text{max}}^{-1})$, where $\lambda_{\text{max}} = \max(\|\mathbf{A}^{\text{ESN}}\|, \lambda_{\text{dep}})$. Then the trained system $\hat{H}_{\hat{\mathbf{W}}}$ satisfies the learning error bound

$$\mathbb{E}[|H(\bar{\mathbf{Z}}) - \hat{H}_{\hat{\mathbf{W}}}(\bar{\mathbf{Z}})|^2]^{1/2} \leq C_{\text{approx}} \left(\lambda^{\frac{N}{d}} + \|\mathbf{A}^{\text{ESN}}\|^T + \frac{1}{N^{\frac{1}{2}}} \right) + C_{\text{est}} \left(RN^{\frac{1}{2}} \frac{\sqrt{\log(n)}}{\sqrt{n}} \right)^{\frac{1}{2}} \quad (6)$$

where $\bar{\mathbf{Z}}$ is an independent copy of \mathbf{Z} and $C_{\text{approx}}, C_{\text{est}}$ are explicitly given and not depending on N, n .

Thank you!

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Appendix Setup I: Sufficiently regular functionals

Consider an unknown functional $H^*: (\mathbb{R}^d)^{\mathbb{Z}_-} \rightarrow \mathbb{R}^m$ and a random input signal \mathbf{Z} (valued in $B_M(0)^{\mathbb{Z}_-}$). The goal is to approximate $H^*(\mathbf{Z})$.

- Key examples:

- $H^*(\mathbf{Z}) = \mathbf{X}_0^*$, where (for a suitable $F^*: \mathbb{R}^{N^*} \times \mathbb{R}^d \rightarrow \mathbb{R}^{N^*}$)

$$\mathbf{X}_t^* = F^*(\mathbf{X}_{t-1}^*, \mathbf{Z}_t), \quad t \in \mathbb{Z}_-.$$

- $H^*(\mathbf{Z}) = \mathbb{E}[\mathbf{Z}_1 | \mathbf{Z}_0, \mathbf{Z}_{-1}, \dots]$.

- Assumptions:

- H^* is d_w -Lipschitz-continuous for some summable weighting sequence w , that is, there exists $L > 0$ such that for all $\mathbf{v}, \mathbf{u} \in B_M(0)^{\mathbb{Z}_-}$

$$\|H^*(\mathbf{v}) - H^*(\mathbf{u})\| \leq L \left[\sum_{t \in \mathbb{Z}_-} w_t \|\mathbf{v}_t - \mathbf{u}_t\|^2 \right]^{1/2}.$$

- For all $T \in \mathbb{N}$ the truncated function(al) $H_T^*: (\mathbb{R}^d)^{T+1} \rightarrow \mathbb{R}^m$, $H_T^*(\mathbf{z}_0, \dots, \mathbf{z}_{-T}) = H^*(\mathbf{z}_0, \dots, \mathbf{z}_{-T}, 0, \dots)$ is sufficiently smooth and integrable (e.g. Sobolev-regularity $W^{2,2}(\mathbb{R}^{d(T+1)})$).

Appendix Setup II: Linear reservoir, random neural network readout

Consider learning based on a recurrent neural network with ReLU activation function and randomly generated $\mathbf{A}, \mathbf{S}, \mathbf{c}, \zeta$ (independent of \mathbf{Z}).

- The input signal $\mathbf{Z} \in (\mathbb{R}^d)^{\mathbb{Z}_-}$ is mapped to the output signal $\mathbf{Y} \in (\mathbb{R}^m)^{\mathbb{Z}_-}$ via

$$\begin{aligned}\mathbf{X}_t &= \sigma_1(\mathbf{S}\mathbf{X}_{t-1} + \mathbf{c}\mathbf{Z}_t), \\ \mathbf{Y}_t &= \mathbf{W}\sigma_2(\mathbf{A}\mathbf{X}_t + \zeta), \quad t \in \mathbb{Z}_-. \end{aligned} \tag{7}$$

- $\sigma_1(x) = x$, $\sigma_2(x) = \max(x, 0)$.
- Each of the N rows of \mathbf{A} is generated (i.i.d.) randomly from uniform distribution in $B_R(0) \subset \mathbb{R}^{d(T+1)}$.
- The entries of ζ are generated i.i.d. uniformly on $[-MR, MR]$.
- \mathbf{S}, \mathbf{c} are (random) matrices with $\lim_{k \rightarrow \infty} \|\mathbf{S}^k\|_2 = 0$ and such that $\mathbf{K} = [\mathbf{c} \ \mathbf{S}\mathbf{c} \ \cdots \ \mathbf{S}^T\mathbf{c}]$ has full rank.
- R, T, N can be chosen (to make the bound as small as possible).
- $\mathbf{W} \in \mathbb{R}^{m \times N}$ is trained (linear regression!).

Appendix: Approximation error bound

Theorem (G., Grigoryeva & Ortega [GGO22])

For any sufficiently regular functional there exists a readout \mathbf{W} (a $\mathbb{R}^{1 \times N}$ -valued random variable) such that for any $\delta \in (0, 1)$, with probability $1 - \delta$ the approximation error satisfies

$$\mathbb{E}[|\mathbf{Y}_0 - H^*(\mathbf{Z})|^2 | \mathbf{A}, \mathbf{S}, \mathbf{c}, \zeta]^{\frac{1}{2}} \leq \frac{1}{\delta} \left[\frac{l_1(T, R)^{\frac{1}{2}}}{\sqrt{N}} + l_2(T, R) + l_3(T) \right], \text{ with}$$

$$l_1(T, R) = C_1(\mathbf{S}, \mathbf{c}) \text{RVol}_{d(T+1)}(B_R(0)) \int_{B_R} \max(1, \|u\|^3) |\widehat{H}_T^*(\mathbf{K}^* u)|^2 du,$$

$$l_2(T, R) = |\det(\mathbf{K})| \int_{B_R(0)^c} |\widehat{H}_T^*(\mathbf{K}^* u)| du,$$

$$l_3(T) = LM \left(\sum_{t=T+1}^{\infty} w_{-t} \right)^{1/2} + C_2(\mathbf{S}, \mathbf{c}) \|\mathbf{S}^T\|.$$

Appendix: Weak dependence

Definition

An \mathbb{R}^k -valued random process \mathbf{U} is said to have a causal Bernoulli shift structure, if there exist $q \in \mathbb{N}$, $G: (\mathbb{R}^q)^{\mathbb{Z}_-} \rightarrow \mathbb{R}^k$ measurable and an i.i.d. collection $(\boldsymbol{\xi}_t)_{t \in \mathbb{Z}_-}$ of \mathbb{R}^q -valued random variables such that

$$\mathbf{U}_t = G(\dots, \boldsymbol{\xi}_{t-1}, \boldsymbol{\xi}_t), \quad t \in \mathbb{Z}_-.$$

It is said to have geometric decay, if there exist $C_{\text{dep}} > 0$, $\lambda_{\text{dep}} \in (0, 1)$ such that the weak dependence coefficient $\theta(\tau) := \mathbb{E}[\|\mathbf{U}_0 - \tilde{\mathbf{U}}_0^\tau\|]$ satisfies $\theta(\tau) \leq C_{\text{dep}} \lambda_{\text{dep}}^\tau$ for all $\tau \in \mathbb{N}$, where

$$\tilde{\mathbf{U}}_0^\tau = G(\dots, \tilde{\boldsymbol{\xi}}_{-\tau-1}, \tilde{\boldsymbol{\xi}}_{-\tau}, \boldsymbol{\xi}_{-\tau+1}, \dots, \boldsymbol{\xi}_0) \text{ for } \tilde{\boldsymbol{\xi}} \text{ an independent copy of } \boldsymbol{\xi}.$$