Towards Explainable AI: Significance Tests for Neural Networks

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Introduction

- Neural networks underpin many of the best-performing AI systems, including speech recognizers on smartphones or Google's latest automatic translator
- The tremendous success of these applications has spurred the interest in applying neural networks in a variety of other fields including finance, economics, operations, marketing, medicine, and many others
- In finance, researchers have developed several promising applications in risk management, asset pricing, and investment management

Literature

- First wave: single-layer nets
    - Financial time series: White (1989), Kuan & White (1994)
    - Nonlinearity testing: Lee, White & Granger (1993)
    - Economic forecasting: Swanson & White (1997)
    - Stock market prediction: Brown, Goetzmann & Kumar (1998)
    - Pricing kernel modeling: Bansal & Viswanathan (1993)
    - Option pricing: Hutchinson, Lo & Poggio (1994)
    - Credit scoring: Desai, Crook & Overstreet (1996)
- Second wave: multi-layer nets (deep learning)
    - Mortgages: Sirignano, Sadhwani & Giesecke (2016)
    - Order books: Sirignano (2016), Cont and Sirignano (2018)
    - Portfolio selection: Heaton, Polson & Witte (2016)
    - Returns: Chen, Pelger & Zhu (2018), Gu, Kelly & Xiu (2018)
    - Hedging: Halperin (2018), Bühler, Gonon & Teichmann (2018)
    - Optimal stopping: Becker, Cheridito & Jentzen (2018)
    - Treasury markets: Filipovic, Giesecke, Pelger, Ye (2019)
    - Real estate: Giesecke, Ohlrogge, Ramos & Wei (2019)
    - Insurance: Wüthrich and Merz (2019)

Explainability

- The success of NNs is largely due to their amazing approximation properties, superior predictive performance, and their scalability
- A major caveat however is **model explainability**: NNs are perceived as black boxes that permit little insight into how predictions are being made
- Key inference questions are difficult to answer
  - Which input variables are statistically significant?
  - If significant, how can a variable's impact be measured?
  - What's the relative importance of the different variables?

Explainability matters in practice

This issue is not just academic; it has slowed the implementation of NNs in financial practice, where regulators and other stakeholders often insist on model explainability

- Credit and insurance underwriting (regulated)
  - Transparency of underwriting decisions
- Investment management (unregulated)
  - Transparency of portfolio designs
  - Economic rationale of trading decisions

This paper

- We develop a **pivotal test** to assess the statistical significance of the input variables of a NN
  - Focus on single-layer feedforward networks
  - Focus on regression setting
- We propose a **gradient-based test statistic** and study its asymptotics using nonparametric techniques
  - Asymptotic distribution is a mixture of χ^2 laws
- The test enables one to address key inference issues:
  - Assess statistical significance of variables
  - Measure the impact of variables
  - Rank order variables according to their influence
- Simulation and empirical experiments illustrate the test

Problem formulation

- Regression model $Y = f_0(X) + \epsilon$
  - $X \in \mathcal{X} \subset \mathbb{R}^d$ is a vector of d feature variables with law P
  - $f_0 : \mathcal{X} \to \mathbb{R}$ is an unknown deterministic C^1-function
  - ϵ is an error variable: $\epsilon \perp\!\!\!\perp X, \mathbb{E}(\epsilon) = 0, \mathbb{E}(\epsilon^2) = \sigma^2 < \infty$
- To assess the significance of a variable X_j, we consider sensitivity-based hypotheses:

$$H_0 : \quad \lambda_j := \int_{\mathcal{X}} \left(\frac{\partial f_0(x)}{\partial x_j}\right)^2 d\mu(x) = 0$$

$$H_A : \quad \lambda_j \neq 0$$

Here, μ is a positive weight measure

- A typical choice is $\mu = P$ and then $\lambda_j = \mathbb{E}[(\frac{\partial f_0(X)}{\partial x_j})^2]$

Intuition

- Suppose the function f_0 is linear (multiple linear regression)

$$f_0(x) = \sum_{k=1}^{d} \beta_k x_k$$

  Then $\lambda_j \propto \beta_j^2$, the squared regression coefficient for X_j, and the null takes the form $H_0 : \beta_j = 0$ ($\rightarrow$ t-test)

- In the general nonlinear case, the derivative $\frac{\partial f_0(x)}{\partial x_j}$ depends on x, and $\lambda_j = \int_{\mathcal{X}} (\frac{\partial f_0(x)}{\partial x_j})^2 d\mu(x)$ is a weighted average

Neural network

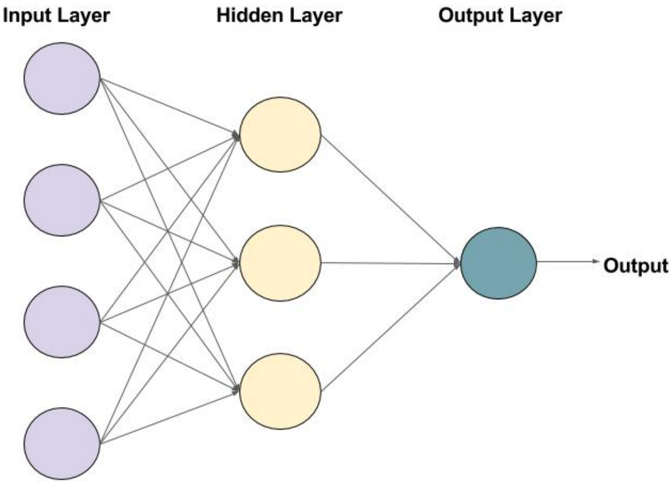
- We study the case where the unknown regression function f_0 is modeled by a single-layer feedforward NN
- A **single-layer NN** f is specified by a bounded *activation function* ψ on $\mathbb{R}$ and the number of *hidden units* K:

$$f(x) = b_0 + \sum_{k=1}^{K} b_k \psi(a_{0,k} + a_k^\top x)$$

  where $b_0, b_k, a_{0,k} \in \mathbb{R}$ and $a_k \in \mathbb{R}^d$ are to be estimated

- Functions of the form f are dense in $C(\mathcal{X})$ (they are *universal approximators*): choosing K large enough, f can approximate f_0 to any given precision

Neural network: d 4 features, K 3 hidden units



Sieve estimator of neural network

- We use n i.i.d. samples (Y_i, X_i) to construct a sieve M-estimator f_n of f for which $K = K_n$ increases with n
- We assume $f_0 \in \Theta =$ class of C^1 functions on d-hypercube $\mathcal{X}$ with uniformly bounded Sobolev norm
- Sieve subsets $\Theta_n \subseteq \Theta$ generated by NNs f with K_n hidden units, bounded L^1 norms of weights, and sigmoid ψ
- The sieve M-estimator f_n is the approximate maximizer of the empirical criterion function $L_n(g) = \frac{1}{n}\sum_{i=1}^{n} l(Y_i, X_i, g)$, where $l : \mathbb{R} \times \mathcal{X} \times \Theta \to \mathbb{R}$, over Θ_n:

$$L_n(f_n) \geq \sup_{g \in \Theta_n} L_n(g) - o_P(1)$$

Neural network test statistic

- The NN **test statistic** is given by

$$\lambda_j^n = \int_{\mathcal{X}} \left(\frac{\partial f_n(x)}{\partial x_j}\right)^2 d\mu(x) = \phi[f_n]$$

- We will use the asymptotic ($n \to \infty$) distribution of λ_j^n for testing the null since a bootstrap approach would typically be too computationally expensive
  1. Asymptotic distribution of f_n
  2. Functional delta method

- In the large-n regime, due to the universal approximation property, we are actually performing inference on the "ground truth" f_0 (**model-free inference**)

Asymptotic distribution of NN estimator

Theorem

Assume that

- $dP = \nu d\lambda$ *for bounded and strictly positive* ν
- *The dimension* K_n *of the NN satisfies* $K_n^{2+1/d} \log K_n = O(n)$,
- *The loss function* $l(y, x, g) = -\frac{1}{2}(y - g(x))^2$.

Then

$$r_n(f_n - f_0) \Longrightarrow h^\star$$

in $(\Theta, L^2(P))$ *where*

$$r_n = \left(\frac{n}{\log n}\right)^{\frac{d+1}{2(2d+1)}}$$

and $h^\star$ *is the argmax of the Gaussian process* $\{\mathbb{G}_f : f \in \Theta\}$ *with mean zero and* $Cov(\mathbb{G}_s, \mathbb{G}_t) = 4\sigma^2 \mathbb{E}(s(X)t(X))$.

Comments

- r_n is the **estimation rate** of the NN (Chen and Shen (1998)):

$$\mathbb{E}_X[(f_n(X) - f_0(X))^2] = O_P(r_n^{-1})$$

  assuming the number of hidden units K_n is chosen such that $K_n^{2+1/d} \log K_n = O(n)$
- Proof uses empirical process arguments
  - Estimation rate implies tightness of $h_n = r_n(f_n - f_0)$
  - Rescaled and shifted criterion function converges weakly to Gaussian process
  - Gaussian process has a unique maximum at $h^\star$
  - Argmax continuous mapping theorem

Asymptotic distribution of test statistic

Theorem

Under the conditions of Theorem 1 and the null hypothesis,

$$r_n^2 \lambda_j^n \Longrightarrow \int_{\mathcal{X}} \left(\frac{\partial h^\star(x)}{\partial x_j} \right)^2 d\mu(x)$$

Empirical test statistic

Theorem

Assume $\mu = P$ so that the test statistic

$$\lambda_j^n = \mathbb{E}_X\left[\left(\frac{\partial f_n(X)}{\partial x_j}\right)^2\right].$$

Under the conditions of Theorem 1 and the null hypothesis, the empirical test statistic satisfies

$$r_n^2 n^{-1}\sum_{i=1}^{n}\left(\frac{\partial f_n(X_i)}{\partial x_j}\right)^2 \Longrightarrow \mathbb{E}_X\left[\left(\frac{\partial h^\star(X)}{\partial x_j}\right)^2\right]$$

Identifying the asymptotic distribution

Theorem

Take $\mu = P$. Let $\{\phi_i\}$ be an orthonormal basis of Θ. If that basis is C^1 and stable under differentiation, then

$$\mathbb{E}_X\left[\left(\frac{\partial h^\star(X)}{\partial x_j}\right)^2\right] = \frac{B^2}{\sum_{i=0}^\infty \frac{\chi_i^2}{d_i^2}} \sum_{i=0}^\infty \frac{\alpha_{i,j}^2}{d_i^4}\chi_i^2,$$

where $\{\chi_i^2\}$ are i.i.d. samples from the chi-square distribution, and where $\alpha_{i,j} \in \mathbb{R}$ satisfies $\frac{\partial \phi_i}{\partial x_j} = \alpha_{i,j}\phi_{k(i)}$ for some $k : \mathbb{N} \to \mathbb{N}$, and the d_i's are certain functions of the $\alpha_{i,j}$'s.

Implementing the test

- Truncate the infinite sum at some finite order N
- Draw samples from the χ^2 distribution to construct a sample of the approximate limiting law
- Repeat m times and compute the empirical quantile $Q_{N,m}$ at level $\alpha \in (0,1)$ of the corresponding samples
  - If $m = m_N \to \infty$ as $N \to \infty$, then Q_{N,m_N} is a consistent estimator of the true quantile of interest
- Reject H_0 if $\lambda_j^n > Q_{N,m_N}(1-\alpha)$ such that the test will be asymptotically of level α:

$$\mathbb{P}_{H_0}\left(\lambda_j^n > Q_{N,m_N}(1-\alpha)\right) \leq \alpha$$

Simulation study

- 8 variables:

$$X = (X_1, \ldots, X_8) \sim U(-1, 1)^8$$

- Ground truth:

$$Y = 8 + X_1^2 + X_2X_3 + \cos(X_4) + \exp(X_5X_6) + 0.1X_7 + \epsilon$$

  where $\epsilon \sim N(0, 0.01^2)$ and X_8 has no influence on Y

- Training (via TensorFlow): 100,000 samples (Y_i, X_i)
  Validation, Testing: 10,000 samples each
- Out-of-sample MSE:

Model	**Mean Squared Error**
NN with $K = 25$	$3.1 \cdot 10^{-4} \sim \mathrm{Var}(\epsilon)$
Linear Regression	0.35

Linear model fails to identify significant variables

Variable	**coef**	**std err**	**t**	$P > \|t\|$
const	**10.2297**	0.002	5459.250	**0.000**
1	-0.0031	0.003	-0.964	0.335
2	0.0051	0.003	1.561	0.118
3	-0.0026	0.003	-0.800	0.424
4	0.0003	0.003	0.085	0.932
5	0.0016	0.003	0.493	0.622
6	-0.0033	0.003	-1.035	0.300
7	**0.0976**	0.003	30.059	**0.000**
8	-0.0018	0.003	-0.563	**0.573**

Only the intercept and the linear term $0.1X_7$ are identified as significant. The irrelevant X_8 is correctly identified as insignificant.

NN test statistic (5% level; 100 experiments; Fourier basis)

Variable	**Test Statistic**	**Power/Size**
1	1.310	1
2	0.332	1
3	0.331	1
4	0.267	1
5	0.480	1
6	0.479	1
7	$\mathbf{1.010 \cdot 10^{-2}}$ $(= 0.1^2)$	1
8	$4.200 \cdot 10^{-6}$	$\mathbf{0.13} > 0.05$

- Size: asymptotic distribution tends to underestimate the variance of the finite sample distribution of the test statistic
- Efficiency: `gradient` (TensorFlow), no re-fitting required
- Robustness: insensitive to correlated feature data

Application: House price valuation

- **Data:** 120+ million housing sales from county registrar of deed offices across the US (source: CoreLogic)
- **Sample period:** 1970 to 2017
- **Geographical area:** Merced County, CA; 76,247 samples
- **Prediction** of $Y = \log$ sale price
- **Variables** $X (d = 68)$: Bedrooms, Full_Baths, Last_Sale_Amount, N_Originations, N_Past_Sales, Sale_Month, SqFt, Stories, Tax_Amount, Time_Since_Prior_Sale, etc.
- Training and gradients via TensorFlow, Adam
- Validation (70/20/10 split): $K = 150$ nodes, L_1 weight 10^{-5}
- Test MSE is 0.45

Application: House price valuation

Top 10 significant (5%) variables (out of 68)

Variable Name	**Test Statistic**
Last_Sale_Amount	1.640
Tax_Land_Square_Footage	1.615
Sale_Month_No	1.340
Tax_Amount	0.383
Last_Mortgage_Amount	0.104
Tax_Assd_Total_Value	0.081
Tax_Improvement_Value_Calc	0.072
Tax_Land_Value_Calc	0.069
Year_Built	0.068
SqFt	0.056
...	...

Conclusion

- We develop a computationally efficient, pivotal significance test for neural networks
  - Assess the impact of feature variables on the prediction
  - Rank variables according to their predictive importance
- This opens up a broader range of applications of NNs in financial practice
- Ongoing work
  - Treatment of NN classifiers and deep networks
  - Cross derivatives for testing interactions between variables
  - Alternative approaches

Example

- Suppose the elements of X are i.i.d. uniform on $[-1, 1]$
- Using the Fourier basis, the limiting distribution takes the form

$$\frac{B^2}{\sum_{n\in\mathbb{N}^d} \frac{\chi_n^2}{d_n^2}} \sum_{n\in\mathbb{N}^d} \frac{n_j^2\pi^2}{d_n^4}\chi_n^2,$$

  - $n = (n_1, n_2 \ldots, n_j, \ldots, n_d)$
  - $d_n^2 = \sum_{|\alpha|\le\lfloor\frac{d}{2}\rfloor+2} \prod_{k=1}^{d}(n_{n_k}\pi)^{2\alpha_k}$
  - $\{\chi_n^2\}_{n\in\mathbb{N}^d}$ are i.i.d. chi-square variables

Computing the asymptotic distribution

- We note that Θ is a subspace of the Hilbert space $L^2(P)$ which admits an orthonormal basis $\{\phi_i\}_{i=0}^{\infty}$
- If this basis is C^1 and stable under differentiation, i.e. if there are a real $\alpha_{i,j}$ and a mapping $k : \mathbb{N} \to \mathbb{N}$ such that

$$\frac{\partial \phi_i}{\partial x_j} = \alpha_{i,j} \phi_{k(i)},$$

then there exists an invertible operator D such that

$$\|f\|_{k,2}^2 = \|Df\|_{L^2(P)}^2 = \sum_{i=0}^{\infty} d_i^2 \langle f, \phi_i \rangle_{L^2(P)}^2$$

where the $d_i's$ are certain functions of the $\alpha_{i,j}$'s