AI for Statistical Analysis

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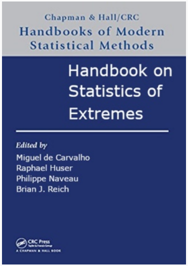
Oct 31, 2025

Outline

- Part I: Basics of deep learning. Background, foundations, rules of thumb, common applications.
- Part II: Using deep learning for statistical analysis. Time series analysis, quantile regression, density estimation, amortized inference for intractable models
- Part III: Further topics. Ongoing research avenues, curios, and resources.

Outline



- Much of the content in parts I and II is based on an AI for extremes short course that Jordan Richards (Edinburgh), Likun Zhang (Mizzou) and I ran during the Contemporary Advances in Statistics of Extremes workshop held at Mizzou in June 2025.
- Deep learning has seen a lot of adoption in the extremes community (keep an eye out for the upcoming handbook!)
- Vignette at `https://github.com/reetamm/AI4stats`.

Preliminaries: Deep learning packages

- The two most popular deep learning packages are `tensorflow` (Abadi et al., 2015) and `torch` (Paszke et al., 2017)
- `tensorflow` was written in Python, while `torch` was written in `C++` with the python version known as `pytorch`
- For the most part, their development happens on `Python`, and hundreds (if not more?) packages use them as their basis
- `tensorflow` has a higher level API called `keras`, which simplifies a lot of the technical aspects.
- `torch` has something similar, called `luz`.
- Both `tensorflow/keras` and `torch/luz` are available on `R`, but their implementations couldn't be more different.
- `tf` on `R` needs `Python`, while `torch` doesn't.

keras vs. torch on R

	`keras`	`torch`
Ease of installation	Complicated	Straightforward
Features	Several Python packages available through reticulate or conda	Limited to packages developed on R
Accessibility	keras makes things easy	Slowly getting better
GPU support	Yes	Yes
Overhead	High on personal systems, but easy to run on Google Colab	Harder to run on Colab, but easy on personal devices

- `tf/keras` on `R` is just a wrapper of the `Python` library made possible by `reticulate`
- Since Google Colab already has Python, it bypasses much of the difficulty and allows the use of `keras3` with relative ease.
- However, it does not support the older `keras` package any more.

Part I: Basics of deep learning

Regression: General Setting

Given:

- Response variable Y (often in $\mathbb{R}$, but could also be discrete classes);
- Covariates $X \in \mathbb{R}^q$.

We are interested in learning some **estimand** that describes the conditional distribution of $Y \mid \mathbf{X} = \mathbf{x}$.

Typical estimands of interest are:

- Class probabilities: $\Pr\{Y = k | \mathbf{X} = \mathbf{x}\}$ for $k \in \mathbb{N}$;
- Expectation: $\mathbb{E}[Y | \mathbf{X} = \mathbf{x}]$;
- Quantiles: $Q_x(\tau) = \inf\{y : F_{Y|\mathbf{X}}(y|x) \geq \tau\}$ for $\tau \in (0, 1)$;
- "Parameters" of $F_{Y|\mathbf{X}}$. Can include parameters in the standard finite-dimensional sense, but may also be interested in semi-/non-parametric model for $F_{Y|\mathbf{X}}$.

Regression: How do we estimate these parameters?

Set up an estimable model $\mathbf{m} : \mathbb{R}^q \mapsto \boldsymbol{\Theta}$:

- Let $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ contain your estimands of interest.
- Setup a function $\mathbf{m}$ that maps your covariates $\mathbf{x}$ to $\boldsymbol{\theta}$, i.e., $\boldsymbol{\theta}(\mathbf{x}) := \mathbf{m}(\mathbf{x})$.
- Get yourself some data $\{(y_i, \mathbf{x}_i)\}_{i=1}^n$.

Estimate $\mathbf{m}$ via minimisation of some loss or cost function:

- Class probabilities: binary cross-entropy;
- Expectation: MSE $n^{-1} \sum_{i=1}^n (y_i - \theta(\mathbf{x}_i))^2$
- Quantiles: Pinball loss $n^{-1} \sum_{i=1}^n (y_i - \theta(\mathbf{x}_i))(\tau - \mathbb{1}\{y_i < \theta(\mathbf{x}_i)\})$;
- $F_{Y|\mathbf{X}}$. Associated negative log-likelihood.

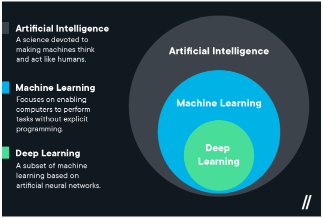
For example, an estimate for the conditional expectation function, say $\widehat{\theta(\mathbf{x})}$, is the minimiser

$$\widehat{\theta(\mathbf{x})} \in \arg\min_{\mathbf{m} \in \mathcal{M}} \frac{1}{n} \sum_{i=1}^{n} (y_i - \mathbf{m}(\mathbf{x}_i))^2,$$

where $\mathcal{M}$ is some appropriate space of estimable functions.

But what should $\mathcal{M}$ look like?

Machine learning

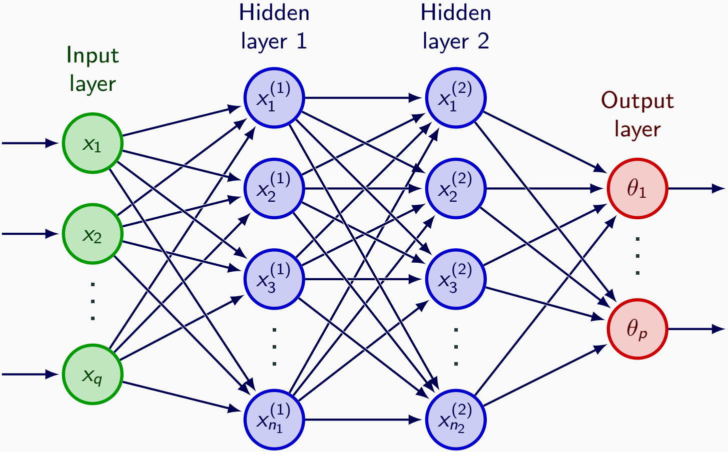


- The **fundamental** difference between statistics and AI/ML/DL is the complexity of $\mathbf{m}(\cdot)$.
- Traditional statistics want $\mathbf{m}(\cdot)$ simple, e.g., linear, parametric, splines, so that estimates are interpretable.
- ML/DL wants flexibility in $\mathbf{m}(\cdot)$.
- Other key ideas - optimisation, regularisation, testing - tend to be the same.

The **deep** in Deep learning comes from the depth of **m**:

- We represent **m** as a neural network. This is just a composition of **layers** of simple, differentiable operations.
- There are lots of different choices of operations, which give rise to different types of neural network. Today, we focus on the standard feed-forward multi-layered perceptron

Deep learning



The neural network $\mathbf{m}_{\psi}$ is constructed as a composition of $L \in \mathbb{N}$ *hidden layers*, $\mathbf{m}^{(l)}$ for $l = 1, \ldots, L$, and an *output/final* layer, $\mathbf{m}^{(L+1)}$, such that $\mathbf{m}_{\psi}(\cdot) := \mathbf{m}^{(L+1)} \circ \cdots \circ \mathbf{m}^{(1)}(\cdot)$.

- ψ contains all the estimable parameters (weights and biases);
- the neural network has the hierarchical structure

$$
\begin{aligned}
\mathbf{x}^{(1)} :=& \mathbf{m}^{(1)}(\mathbf{x}) = \mathbf{a}^{(1)}\left(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}\right), \\
\mathbf{x}^{(2)} :=& \mathbf{m}^{(2)}(\mathbf{x}^{(1)}) = \mathbf{a}^{(2)}\left(\mathbf{W}^{(2)}\mathbf{x}^{(1)} + \mathbf{b}^{(2)}\right), \\
&\vdots \\
\mathbf{x}^{(L)} :=& \mathbf{m}^{(L)}(\mathbf{x}^{(L-1)}) = \mathbf{a}^{(L)}\left(\mathbf{W}^{(L)}\mathbf{x}^{(L-1)} + \mathbf{b}^{(L)}\right), \\
\boldsymbol{\theta}(\mathbf{x}) :=& \mathbf{m}^{(L+1)}(\mathbf{x}^{(L)}) = \mathbf{a}^{(L+1)}\left(\mathbf{W}^{(L+1)}\mathbf{x}^{(L)} + \mathbf{b}^{(L+1)}\right).
\end{aligned}
$$

Activation functions

Activation functions provide flexibility by making the layers non-linear.

Popular choices includes:

- ReLU: $\mathbf{a}(\mathbf{x})_j = \max(x_j, 0)$
- sigmoid: $\mathbf{a}(\mathbf{x})_j = \exp(x_j)/(1 + \exp(x_j))$
- tanh
- eLU and leaky ReLU
- softmax: $\mathbf{a}(\mathbf{x}) = (\frac{\exp(x_1)}{\sum_i \exp(x_i)}, \frac{\exp(x_2)}{\sum_i \exp(x_i)}, \dots)$

Some common types of layers

- Dense layer
- Convolutional layer
- Maxpooling layer
-

Training models

Models are trained by solving the empirical risk minimisation problem

$$\widehat{\boldsymbol{\psi}} \in \arg\min_{\boldsymbol{\psi}} \frac{1}{n} \sum_{i=1}^{n} \ell\{y_i; \mathbf{m}_{\boldsymbol{\psi}}, (\mathbf{x}_i)\},$$

where ℓ is our loss function.

In **statistics**, this would be achieved using gradient descent, via the update

$$\boldsymbol{\psi} \leftarrow \boldsymbol{\psi} - \frac{\lambda}{n} \sum_{i=1}^{n} \boldsymbol{\nabla}_{\boldsymbol{\psi}} \ell\{y_i, \mathbf{m}_{\boldsymbol{\psi}}(\mathbf{x}_i)\}, \tag{1}$$

where $\lambda > 0$ is a tunable learning rate and $\boldsymbol{\nabla}_{\boldsymbol{\psi}}$ denotes the differential operator with respect to entries in $\boldsymbol{\psi}$.

Training deep models

In **deep learning**, where n is typically large, a more economical approach is to update over individual observations (SGD), using the rule

$$\boldsymbol{\psi} \leftarrow \boldsymbol{\psi} - \lambda \boldsymbol{\nabla}_{\boldsymbol{\psi}} \ell\{y_i, \mathbf{g}_{\boldsymbol{\psi}}(\mathbf{x}_i)\}, \qquad i = 1, \ldots, n. \tag{2}$$

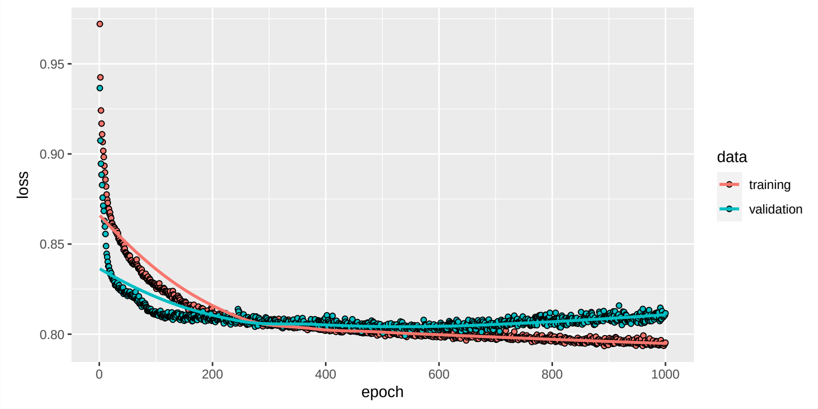
Neural networks are usually trained using an algorithm that falls in-between gradient descent and true SGD, which is called *mini-batch SGD*. In this case, all samples are split into n_b mini-batches of equal size, and n_b updates are performed for every **epoch** of the training scheme.

Usually, $\boldsymbol{\nabla}_{\boldsymbol{\psi}}$ is tractable and fast-to-compute via **backpropagation**. This is because the neural network model is a composition of simple differentiable operations.

Regularisation: Training/validation/testing

Due to their large number of parameters, neural networks are prone to overfitting. It's necessary to use **validation/testing** to assess overfitting.

- Subset the data into training, validation, and testing.
- Each set has a different purpose:
    - The model is **trained** on the training data. This is used to update the weights and biases.
    - We **validate** the model on the validation data. Typically used for model selection.
    - To get a truly unbiased evaluation of the model fit and to compare amongst different models, we **test** the model on test data.



loss
0.95
0.90
0.85
0.80
0
200
400
600
800
1000
epoch
data
training
validation

Regularisation/numerics

Other forms of regularisation to consider:

- Weight penalties (think LASSO or ridge)
- Random weight initialization
- Dropout
- Sharing weights*
- Early-stopping* and checkpoints*

Some numerical aspects:

- Pre-training*
- Standardising input data*
- Parameter dependent support
- Optimizing architecture/training scheme (please don't ask about this)

Part II: Deep Learning for Statistical Analysis

Deep GPD regression

We now use these ideas to perform deep GPD regression. We perform a **two-stage** estimation procedure:

- Use the tilted loss to estimate $u(\mathbf{x})$ as the τ-quantile of $Y \mid \mathbf{x} = \mathbf{x}$ (for τ close to one).
- Model conditional excesses $(Y - u(\mathbf{x})) \mid (\mathbf{X} = \mathbf{x})$ as $\text{GPD}(\sigma_u(\mathbf{x}), \xi(\mathbf{x}))$.

The latter stage follows via maximum likelihood and we consider three different models for $(\sigma_u(\mathbf{x}), \xi(\mathbf{x}))$.

Semi-parametric quantile regression (SPQR)

Estimating entire densities

- Our goal almost always is to make probability statements based on a fitted model
- However, sometimes we *don't* want to assume a parametric form of the density
- In that case, we need:
  - A non/semi-parametric way to represent the density
  - A loss function which evaluates the (usual negative log-likelihood) loss between the response y_i and the estimates $\pi(x_i)$
- SPQR does this using an $M-$spline representation of continuous density functions

SPQR

SPQR represents a continuous distribution $Y|X$ as:

$$f(y|x) = \sum_{k=1}^{K} \pi_k(x) M_k(y)$$

- $\{\pi_k\}_{k=1}^{K}$ is a vector of probabilities output from a NN
- The loss function is $-\log f(y|x)$
- $M-$splines are rescaled $B-$splines
- $I-$splines are just integrated $M-$splines such that:

$$F(y|x) = \sum_{k=1}^{K} \pi_k(x) I_k(y)$$

- Representation is scale-invariant

The good, the bad, and the next.

While the demo uses `keras`, there *is* a package based on `torch` at `https://github.com/stevengxu/SPQR` (Xu et al., 2022).
Good.

- Supports multi-modal input and various architectures
- Quantile function can be estimated using interpolation
- Can easily make probability statements

Bad.

- $M-$splines are bounded - extrapolation outside the observed range of y not possible

Next up.

- SPQRx (Majumder and Richards, 2025)

Part III: Further topics

Further topics

Machine learning for extreme quantile/extremal regression:

- NN-based methods:
  - GEV: (Cannon, 2010; Vasiliades et al., 2015; Bennett et al., 2015; Richards and Huser, 2024)
  - GPD: (Carreau and Bengio, 2007; Carreau et al., 2009; Carreau and Vrac, 2011; Richards et al., 2023; Allouche et al., 2024; Dahal et al., 2024; Pasche and Engelke, 2024; Majumder and Richards, 2025; Wilson et al., 2022)
  - Other: (Richards and Huser, 2022; Cisneros et al., 2024)
- Classical ML:
  - Random forests: (Taillardat et al., 2019; Gnecco et al., 2024)
  - Regression trees: (Farkas et al., 2021, 2024)
  - Boosting: (Velthoen et al., 2023; Koh, 2023; Koh et al., 2025)

Further topics

Multivariate and spatial models:

- Geometric methods: (Murphy-Barltrop et al., 2024; Mackay et al., 2025; De Monte et al., 2025)
- *d*-max-decreasing NNs: (Hasan et al., 2022)
- Deep compositional spatial models: (Shao et al., 2025)
- Generative methods:
  - Excess-GAN :(Allouche et al., 2025)
  - Ex-GAN: (Bhatia et al., 2021)
  - EV-GAN: (Allouche et al., 2022)
  - GPDflow: (Hu and Castro-Camilo, 2025)
  - EVT-GAN: (Boulaguiem et al., 2022)
  - HT-GAN: (Girard et al., 2024)
  - GP-GAN (Li et al., 2024)
  - Angular simulation: (Wessel et al., 2025)
  - WA-GAN: (Lhaut et al., 2025)
  - VAEs: (Lafon et al., 2023; Zhang et al., 2023)

Further topics

Statistical (unsupervised) learning:

- Clustering: (Janßen and Wan, 2020; Bernard et al., 2013; Saunders et al., 2021; Bador et al., 2015; Rohrbeck and Tawn, 2021; Vignotto et al., 2021; Boulin et al., 2023)
- Dimension reduction: (Chautru, 2015; Drees and Sabourin, 2021; Cooley and Thibaud, 2019)
- Anomaly detection: (Clifton et al., 2014; Rudd et al., 2017; Vignotto and Engelke, 2020)
- Review by Clémençon and Sabourin (2025)

Further topics

Fast inference:

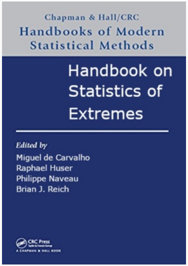
- Neural estimation:
  - Spatio-temporal: (Lenzi et al., 2023; Sainsbury-Dale et al., 2024a,b; Richards et al., 2024; Sainsbury-Dale et al., 2025; Dell'Oro and Gaetan, 2024; Rai et al., 2025; Hector and Lenzi, 2024)
  - Multivariate: (André et al., 2025; Hua, 2025)
  - Univariate: (Rai et al., 2024; Richards et al., 2025)
- Intractable likelihood approximation: (Walchessen et al., 2024; Majumder and Reich, 2023; Majumder et al., 2024)
- Variational inference: (Maceda et al., 2024)
- Dependence classification: (Ahmed et al., 2022; Wixson and Cooley, 2024)

Further topics

Other things to look out for:

- KANs: (de Carvalho et al., 2025)
- Conformal prediction: (Pasche et al., 2025)

Handbook chapters



- Ch11 - Principal Component Analysis for Multivariate Extremes. Cooley, Sabourin, and Wixson.
- Ch12 - Clustering Methods for Multivariate Extremes. Wan and Janßen.
- Ch20 - On the Simulation of Extreme Events with Neural Networks. Allouche, Girard, and Gobet.
- Ch21 - Extreme Quantile Regression with Deep Learning. Richards and Huser.
- Ch26 - Statistics of Extremes for Wildfires. Koh.

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