1 Regression

1.1 Terminology

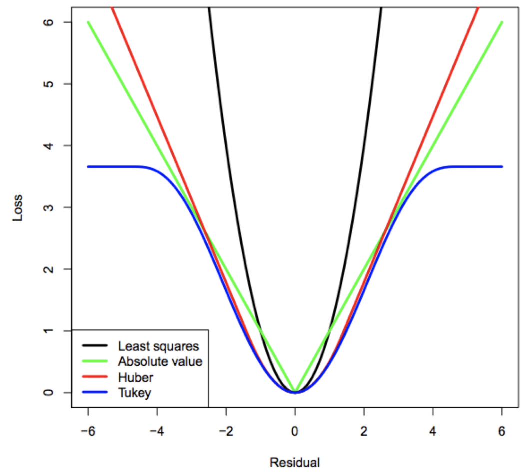
- Data consists of **pairs** $(\mathbf{x}_n, y_n)$, where y_n is the n'th output and x_n is a vector of D inputs. The number of pairs N is the data-size and D is the dimensionality.
- Two goals of regression: **prediction** and **interpretation**
- The regression function: $y_n \approx f_w(\mathbf{x}_n)\ \forall n$
- Regression finds correlation not a causal relationship.
- **Input variables** a.k.a. covariates, independent variables, explanatory variables, exogenous variables, predictors, regressors.
- **Output variables** a.k.a. target, label, response, outcome, dependent variable, endogenous variables, measured variable, regressands.

1.2 Linear Regression

- Assumes linear relationship between inputs and output.
- $y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1} + \ldots + w_D x_{nD} := \tilde{\mathbf{x}}_n^T \tilde{\mathbf{w}}$ contain the additional offset term (a.k.a. bias).
- Given data we learn the weights $\mathbf{w}$ (a.k.a. estimate or fit the model)
- Overparameterisation $D > N$ eg. univariate linear regression with a single data point $y_1 \approx w_0 + w_1 x_{11}$. This makes the task under-determined (no unique solution).

1.3 Loss Functions $\mathcal{L}$

- A loss function (a.k.a. energy, cost, training objective) quantifies how well the model does (how costly its mistakes are).
- $y \in \mathbb{R} \Rightarrow$ desirable for cost to be symmetric around 0 since $\pm$ errors should be penalized equally.
- Cost function should penalize "large" mistakes and "very large" mistakes similarly to be robust to outliers.
- Mean Squared Error:
$\mathrm{MSE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}[y_n - f_{\mathrm{w}}(\mathbf{x}_n)]^2$
not robust to outliers.
- Mean Absolute Error:
$\mathrm{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}|y_n - f_{\mathrm{w}}(\mathbf{x}_n)|$
- Convexity: a function is convex iff a line segment between two points on the function's graph always lies above the function.
- Convexity: a function $h(\mathbf{u}), \mathbf{u} \in \mathbb{R}^D$ is convex if $\forall\ \mathbf{u}, \mathbf{v} \in \mathbb{R}^D, 0 \le \lambda \le 1$:
$h(\lambda\mathbf{u} + (1-\lambda)\mathbf{v}) \le \lambda h(\mathbf{u}) + (1-\lambda)h(\mathbf{v})$
Strictly convex if $\le \Rightarrow <$
- Convexity, a desired computational property: A strictly convex function has a unique global minimum $\mathbf{w}^*$. For convex functions, every local minimum is a global minimum.
- Sums of convex functions are also convex $\Rightarrow$ MSE combined with a linear model is convex in $\mathbf{w}$.
- Proof of convexity for MAE:
$\mathrm{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}_n(\mathbf{w}), \mathcal{L}_n(\mathbf{w}) = |y_n - f_{\mathrm{w}}(\mathbf{x}_n)|$
$\mathcal{L}_n(\lambda w_1 + (1-\lambda)w_2) \le \lambda\mathcal{L}_n(w_1) + (1-\lambda)\mathcal{L}_n(w_2)$
$|y_n - x_n^T(\lambda w_1 + (1-\lambda)w_2)| \le \lambda|y_n - x_n^T w_1| + (1-\lambda)|y_n - x_n^T w_2|$
$(1-\lambda) \ge 0 \Rightarrow (1-\lambda)|y_n - x_n^T w_2| = |(1-\lambda)y_n - (1-\lambda)x_n^T w_2|$
$a = \lambda y_n - \lambda x_n^T w_1, b = (1-\lambda)y_n - (1-\lambda)x_n^T w_2$
$a + b = y_n - x_n^T(\lambda w_1 + (1-\lambda)w_2)$
$|a+b| \le |a| + |b| \Rightarrow \mathcal{L}_n(\mathbf{w})$ convex $\Rightarrow \mathrm{MAE}(\mathbf{w})$ convex
- Huber loss:
$\mathcal{H}uber(e) := \begin{cases} \frac{1}{2}e^2 & \text{, if } |e| \le \delta \\ \delta|e| - \frac{1}{2}\delta^2 & \text{, if } |e| > \delta \end{cases}$ convex, differentiable, and robust to outliers but setting δ is not easy.
- Tukey's bisquare loss:
$\frac{\partial\mathcal{L}}{\partial e} := \begin{cases} e\{1 - e^2/\delta^2\}^2 & \text{, if } |e| \le \delta \\ 0 & \text{, if } |e| > \delta \end{cases}$ non-convex, but robust to outliers.



2 Optimisation

- Given $\mathcal{L}(\mathbf{w})$ we want $\mathbf{w}^* \in \mathbb{R}^D$ which minimises the cost: $\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}) \rightarrow$ formulated as an optimisation problem
- Local minimum $\mathbf{w}^* \Rightarrow \exists\epsilon > 0$ s.t.
$\mathcal{L}(\mathbf{w}^*) \le \mathcal{L}(\mathbf{w})\ \forall\mathbf{w}$ with $\|\mathbf{w} - \mathbf{w}^*\| < \epsilon$
- Global minimum $\mathbf{w}^*$, $\mathcal{L}(\mathbf{w}^*) \le \mathcal{L}(\mathbf{w})\ \forall\mathbf{w} \in \mathbb{R}^D$

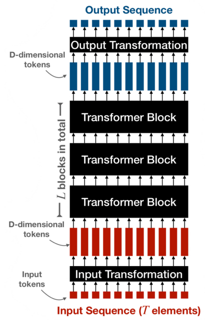
2.1 Smooth Optimisation

3 Transformers

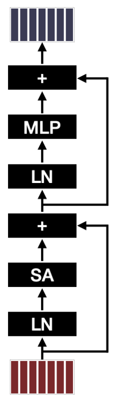
- A transformer is a neural network that iteratively transforms a sequence to another sequence and mixes the information between the sequence elements via self-attention.

3.1 Architecture

- Self-Attention (SA): mixes information between tokens
- Multi-Layer Perceptron (MLP): mixes information within each token
- Skip connections are widely used
- Layer normalization (LN) is usually placed at the start of a residual branch



3.2 Text Token Embeddings



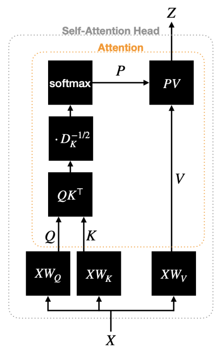
- Tokenization: split the input text into a sequence of input tokens (typically word fragments + some special symbols) according to some pre-defined tokenizer procedure:
- Convert each token ID $i \in \{1, \ldots, N_{vocab}\}$ into a real-valued vector $\mathbf{w}_i \in \mathbb{R}^D$
- This can be seen as a matrix multiplication $\mathbf{W} \cdot \mathbf{e}_i = \mathbf{W}_{:,i} = \mathbf{w}_i$ (with $\mathbf{W} \in \mathbb{R}^{\mathrm{D} \times \mathrm{N_{vocab}}}$)
- $\mathbf{W}$ is learned via backpropagation, along with all other transformer parameters (however, the tokenizer procedure is typically fixed in advance and not learned)
- The whole input sequence of T tokens leads to an input matrix $X \in \mathbb{R}^{T \times D}$

3.3 Attention

- Attention is a function that transforms a sequence of tokens to a new sequence of tokens using a learned input-dependent weighted average
- Input tokens : $V \in \mathbb{R}^{T_{in} \times D}$
- Output tokens : $Z \in \mathbb{R}^{T_{out} \times D}$
- Output tokens are simply a weighted average of the input tokens: $z_i = \sum_{j=1}^{T_i} p_{ij} v_j$ i.e. $Z = PV$
- Weighting coefficients $\mathcal{P} \in [0,1]^{T_{out} \times T_{in}}$ form valid probability distributions over the input tokens $\sum_{j=1}^{T_{in}} p_{ij} = 1$
- Query tokens : $Q \in \mathbb{R}^{T_{out} \times D_K}$
- Key tokens : $K \in \mathbb{R}^{T_{in} \times D_K}$
- Determine weight $p_{i,j}$ based on how simmilar q_i and k_j are.
- Use inner product to obtain raw similarity scores.
- Normalize with softmax (scaled the temperature by $\sqrt{D_K}$) to obtain a probability distribution.
- $P = \mathrm{softmax}\left(\frac{QK^{\mathsf{T}}}{\sqrt{D_K}}\right)$ The softmax is applied on each row independently. Scaling ensures uniformity at initialization and faster convergence

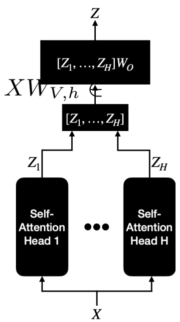
3.4 Self-Attention

- V, K, Q are all derived from the same input token sequence $X \in \mathbb{R}^{T \times D}$
- Values : $V = XW_V \in \mathbb{R}^{T \times D}$, $W_V \in \mathbb{R}^{D \times D}$
- Keys : $K = XW_K \in \mathbb{R}^{T \times D_K}$, $W_K \in \mathbb{R}^{D \times D_K}$
- Queries : $Q = XW_Q \in \mathbb{R}^{T \times D_K}, W_Q \in \mathbb{R}^{D \times D_K}$
- W_Q, W_V, W_K are learned parameters.
- $Z = \mathrm{softmax}\left(\frac{XW_Q W_K^T X^T}{\sqrt{D_K}}\right) XW_V$



3.4.1 Multi-Head Self-Attention

- Run H Self-Attention "heads" in parallel
- $Z_h = \mathrm{softmax}\left(\frac{XW_{Q,h}W_{K,h}^{\mathsf{T}}X^{\mathsf{T}}}{\sqrt{D_K}}\right) XW_{V,h} \in \mathbb{R}^{T \times D_V}$
- $W_{V,h} \in \mathbb{R}^{D \times D_V}$, $W_{K,h} \in \mathbb{R}^{D \times D_K}$, $W_{Q,h} \in \mathbb{R}^{D \times D_K}$
- The final output is obtained by concatenating head-outputs and applying a linear transformation $Z = [Z_1, \ldots, Z_H]W_o$ where $W_O \in \mathbb{R}^{HD_V \times D}$ is learned via backpropagation



3.5 Positional Information

- Attention by itself does not account for the order of input
- incorporate a positional encoding in the network which is a function from the position to a feature vector $pos : \{1, \ldots, T\} \rightarrow \mathbb{R}^D$
- The most basic choice is to add a positional embedding W_{pos} corresponding to each token's position t to the input embedding. $W_{pos} \in \mathbb{R}^{D \times T}$ is learned via backpropagation along with the other parameters

3.6 MLP

- Mixing Information within Tokens
- Apply the same transformation to each token independently: $MLP(X) = \varphi(XW_1)W_2$
- $W_1, W_2 \in \mathbb{R}^{D \times D}$ learned via backprop

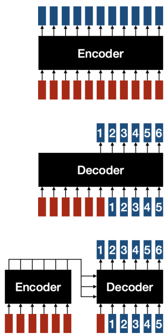
3.7 Output Transformations

- typically simple: linear transformation or a small MLP
- dependent on the task: Single output (e.g.,sequence-level classification): apply an output transformation to a special taskspecific input token or to the average of all tokens. Multiple outputs (e.g., per-token classification): apply an output transformation to each token independently

3.8 Vision Transformer Architecture

- Self-attention is more general than convolution and can potentially express it
- The receptive field is the whole image after just one self-attention layer
- ViTs require more data than CNNs due to their reduced inductive bias in extracting local features
- In many cases, the model attends to image regions that are semantically relevant for classification

3.9 Encoders & Decoders



- Encoders (e.g., classification): They produce a fixed output size and process all inputs simultaneously
- Decoders (e.g., ChatGPT): Auto-regressively sample the next token as $x_{t+1} \sim sofimax(f(x_1, ..., x_t))$ and use it as new input token. Capable of generating responses of arbitrary length.
- Encoder-decoder (e.g., translation): First encode the whole input (e.g., in one language) and then decode to token by token (e.g., in a different language)

4 Adversarial ML

5 This is RGB red text.

For $x \in [r_{i-1}, r_i]$
$r(x) = \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^{m} \tilde{a}_j (x - \tilde{b}_j)_+$

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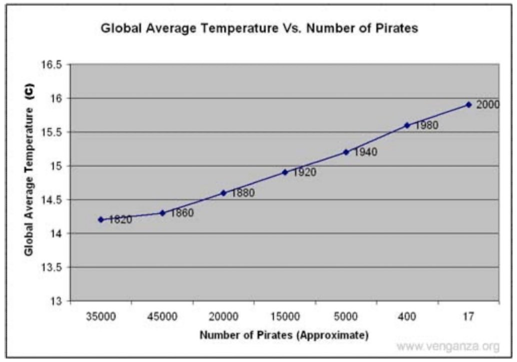

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