Regression

Terminology

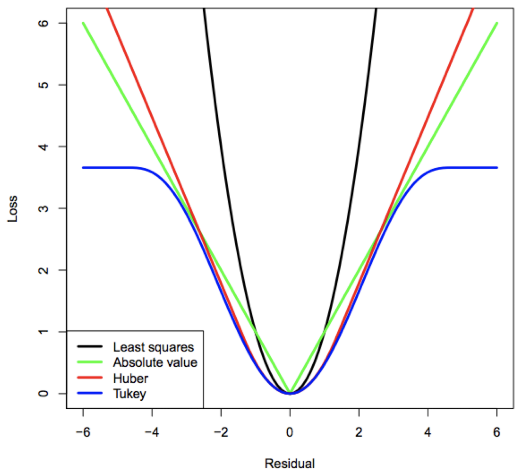
- Data consists of **pairs** $(\mathbf{x}_n, y_n)$, where y_n is the n'th output and x_n is a vector of D inputs. The number of pairs N is the data-size and D is the dimensionality.
- Two goals of regression: **prediction** and **interpretation**
- The regression function: $y_n \approx f_w(\mathbf{x}_n)\ \forall n$
- 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.

Linear Regression

- Assumes linear relationship between inputs and output.
- $y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1} + ... + w_D x_{nD}$ $:= \tilde{\mathbf{x}}_n^T \tilde{\mathbf{w}}$ 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).

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:
$\mathsf{MSE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}[y_n - f_{\mathrm{w}}(\mathbf{x}_n)]^2$
not robust to outliers.
- Mean Absolute Error:
$\mathsf{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}|y_n - f_{\mathrm{w}}(\mathbf{x}_n)|$
- 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:
$\mathsf{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}_n(\mathbf{w}), \mathcal{L}_n(\mathbf{w}) = |y_n - f_{\mathrm{w}}(\mathbf{x}_n)|$
$\mathcal{L}_n(\lambda w_1 + (1-\lambda)w_2) \le \lambda\mathcal{L}_n(w_1) + (1-\lambda)\mathcal{L}_n(w_2)$
$|y_n - x_n^T(\lambda w_1 + (1-\lambda)w_2)| \le \lambda|y_n - x_n^T w_1| + (1-\lambda)|y_n - x_n^T w_2|$
$(1-\lambda) \ge 0 \Rightarrow (1-\lambda)|y_n - x_n^T w_2| = |(1-\lambda)y_n - (1-\lambda)x_n^T w_2|$
$a = \lambda y_n - \lambda x_n^T w_1, b = (1-\lambda)y_n - (1-\lambda)x_n^T w_2$
$a + b = y_n - x_n^T(\lambda w_1 + (1-\lambda)w_2)$
$|a+b| \le |a| + |b| \Rightarrow \mathcal{L}_n(\mathbf{w})$ convex $\Rightarrow \mathsf{MAE}(\mathbf{w})$ 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.



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 $\mathbf{w}^*$, $\mathcal{L}(\mathbf{w}^*) \le \mathcal{L}(\mathbf{w})\ \forall\mathbf{w} \in \mathbb{R}^D$

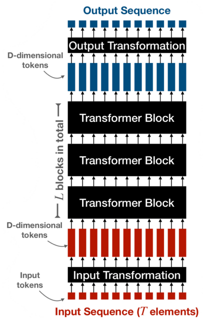
Smooth Optimisation

Transformers

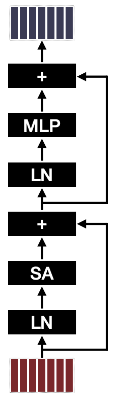
- A transformer is a neural network that iteratively transforms a sequence to another sequence and mixes the information between the sequence elements via self-attention.

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



Text Token Embeddings

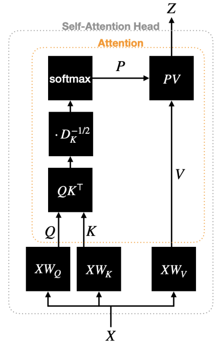


- Tokenization: split the input text into a sequence of input tokens (typically word fragments + some special symbols) according to some predefined tokenizer procedure:
- Convert each token ID $i \in \{1, ..., N_{vocab}\}$ into a real-valued vector $\mathbf{w}_i \in \mathbb{R}^D$
- This can be seen as 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 $X \in \mathbb{R}^{T \times D}$

Attention

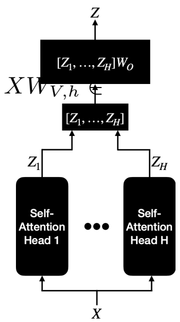
- Attention is a function that transforms a sequence of tokens to a new sequence of tokens using a learned input-dependent weighted average
- Input tokens : $V \in \mathbb{R}^{T_{in} \times D}$
- Output tokens : $Z \in \mathbb{R}^{T_{out} \times D}$
- Output tokens are simply a weighted average of the 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.
- $P = \text{softmax}\left(\frac{QK^\top}{\sqrt{D_K}}\right)$ The softmax is applied on each row independently. Scaling ensures uniformity at initialization and faster convergence

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.
- $Z = \text{softmax}\left(\frac{XW_Q W_K^T X^T}{\sqrt{D_K}}\right) XW_V$

Multi-Head Self-Attention



- Run H Self-Attention "heads" in parallel
- $Z_h = \text{softmax}\left(\frac{XW_{Q,h}W_{K,h}^\top X^\top}{\sqrt{D_K}}\right) XW_{V,h} \in \mathbb{R}^{T \times D_V}$
- $W_{V,h} \in \mathbb{R}^{D \times D_V}$, $W_{K,h} \in \mathbb{R}^{D \times D_K}$, $W_{Q,h} \in \mathbb{R}^{D \times D_K}$
- 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

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 $pos : \{1, ..., T\} \rightarrow \mathbb{R}^D$
- 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

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

Output Transformations

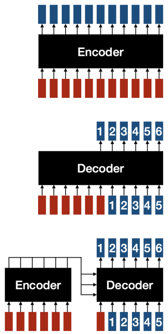
- typically simple: linear transformation or a small MLP

- 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

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

Encoders & Decoders



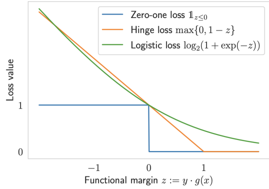
- Encoders (e.g., classification): They produce a fixed output size and process all inputs simultaneously
- Decoders (e.g., ChatGPT): Auto-regressively sample the next token as $x_{t+1} \sim sofimax(f(x_1, ..., x_t))$ and use it as new input token. Capable of generating responses of arbitrary length.
- 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)

Adversarial ML

- We don't understand how NN models generalize and react to shifts in the distribution of data (i.e., distribution shifts)
- Classification problem: $(X, Y) \sim \mathcal{D}$, Y with range $\{-1, 1\}$
- Standard risk: average zero-one loss over X: $R(f) = \mathbb{E}_{\mathcal{D}}\left[1_{f(X) \neq Y}\right] = \mathbb{P}_{\mathcal{D}}\left[f(X) \neq Y\right]$ i.e. minimise proba of wrong prediction.
- Adversarial risk: average zero-one loss over small, worst-case perturbations of X: $R_\varepsilon(f) = \mathbb{E}_{\mathcal{D}}\left[\max_{\hat{x}, \|\hat{x}-X\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y}\right]$

Generating adversarial examples

- Task: given an input (x, y) and a model $f : \mathcal{X} \to \{-1, 1\}$ find an input $\hat{x}$ s.t.: a) $\|\hat{x} - x\| \leq \varepsilon$ b) the model f makes a mistake on it.
- Trivial case: x already missclassified → no action required
- General case: find $\hat{x}$ such that at $f(\hat{x}) \neq y$ and $||\hat{x} - x|| \leq \varepsilon$ i.e. $\hat{x} \in B_x(\varepsilon) \cap \{x' f(x') = -y\}$
- Optimization problem with respect to the inputs
- Problem: optimizing the indicator function is difficult: 1) The indicator function 1 is not continuous 2) The NN prediction f outputs discrete class values $\{-1, 1\}$
- Replace the difficult problem involving the indicator with a smooth problem $\max_{\hat{x}, \|\hat{x}-X\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y} \to \max_{\hat{x}, \|\hat{x}-X\| \leq \varepsilon} \ell(yg(\hat{x}))$
- decreasing, margin-based (i.e., dependent on $y * g(x)$) classification losses



White-Box attacks

- Solve $\max_{\hat{x}, \|\hat{x}-X\| \leq \varepsilon} \ell(yg(\hat{x}))$ knowing g
- $\nabla_x \ell(yg(x)) = y\ell'(yg(x)) \nabla_x g(x)$, with $y\ell'(yg(x)) \leq 0$ since classification losses are decreasing.
- Move in direction of $\propto -y \nabla_x g(x)$
- Interpretation $f(x) = \text{sign}(g(x))$: If $y = 1$ we want to decrease $g(x)$ and follow $-\nabla_x g(x)$. If $y = -1$ we want to decrease $g(x)$ and follow $\nabla_x g(x)$
- By using ℓ and not directly $yg(\hat{x})$ it will extend to multi-class classification and robust training.
- linearize the loss $\tilde{\ell}(x) := \ell(yg(x))$

$\max_{\|\hat{x}-x\| \leq \varepsilon} \tilde{\ell}(x)$
$\approx \max_{\|\hat{x}-x\| \leq \varepsilon} \tilde{\ell}(x) + \nabla_x \tilde{\ell}(x)^T (\hat{x} - x)$
$= \tilde{\ell}(x) + \max_{\|\hat{x}-x\| \leq \varepsilon} \nabla_x \tilde{\ell}(x)^T (\hat{x} - x)$
$= \tilde{\ell}(x) + \max_{\|\delta\| \leq \varepsilon} \nabla_x \tilde{\ell}(x)^T \delta$

- We need to maximize the inner product under a norm constraint, i.e. find the optimal local update
- This is a simple problem for which we can get a closed-form solution depending on the norm used to measure the perturbation size $||\delta||$

One-step attack

- Solution for the ℓ_2 norm:

$\delta_2^\star = \varepsilon \cdot \frac{\nabla_x \tilde{\ell}(x)}{||\nabla_x \tilde{\ell}(x)||_2} = -\varepsilon y * \frac{\nabla_x g(x)}{||\nabla_x g(x)||_2} \Rightarrow$
$\hat{x} = x - \varepsilon y \cdot \frac{\nabla_x g(x)}{\|\nabla_x g(x)\|_2}$

- Solution for the ℓ_∞ norm called **Fast Gradient Sign Method**:

$\delta_\infty^\star = \varepsilon \cdot \text{sign}(\nabla_x \tilde{\ell}(x)) = -\varepsilon y \cdot \text{sign}(\nabla_x g(x)) \Rightarrow$
$\hat{x} = x - \varepsilon y \cdot \text{sign}(\nabla_x g(x))$

Multi-step attack

- These updates can be done iteratively and combined with a projection Π on the feasible set (i.e., balls ℓ_2 / ℓ_∞ here)
- Projected Gradient Descent (PGD attack)
- ℓ_2 norm:

$\delta^{t+1} = \Pi_{B_2(e)}[\delta^t + \alpha \cdot \frac{\nabla \tilde{\ell}(x+\delta^t)}{\|\nabla \tilde{\ell}(x+\delta^t)\|_2}]$

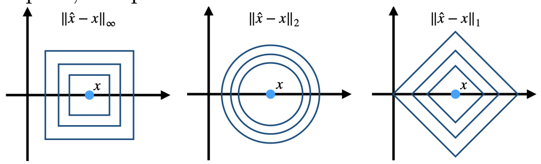
$$\Pi_{B_2(\varepsilon)}(\delta) = \begin{cases} \varepsilon \cdot \delta / \|\delta\|_2, & \text{if } \|\delta\|_2 \geq \varepsilon \\ \delta \text{ otherwise} \end{cases}$$

- ℓ_∞ norm:

$$\delta^{t+1} = \Pi_{B_\infty(\varepsilon)}\left[\delta^t + \alpha \cdot \text{sign}(\nabla \tilde{\ell}(x + \delta^t))\right],$$

$$\Pi_{B_\infty(\varepsilon)}(\delta)_i = \begin{cases} \varepsilon \cdot \text{sign}(\delta_i), & \text{if } |\delta_i| \geq \varepsilon \\ \delta_i \text{ otherwise} \end{cases}$$

- the gradients are computed by backprop w.r.t. inputs, not parameters!



Black-box attacks

- We don't know $g(x)$
- Obtaining a surrogate model can be costly and there is no guarantee of success
- Query-based methods often require a lot of queries (10k-100k), easy to restrict access for the attacker!

Query-based gradient estimation

- Score-based: we can query the continuous model scores $g(x) \in \mathbb{R}$. We can approximate the gradient by using the finite difference formula: $\nabla_x g(x) \approx \sum_{i=1}^d \frac{g(x+\alpha e_i) - g(x)}{\alpha} e_i$
- Decision-based: we can query only the predicted class $f(x) \in \{-1, 1\}$, similar techniques can be adapted for the decision-based case.

Transfer Attacks

- Train a similar surrogate model $\hat{f} \approx f$ on similar data
- Model stealing (query f given some unlabeled inputs $\{x_n, f(x_n)\}_{n=1}^N$) can facilitate transfer attacks.

Adversarial training

- Adversarial training: the goal is to minimize the adversarial risk:

$\min_\theta R_\varepsilon(f_\theta) = \mathbb{E}_{\mathcal{D}}\left[\max_{\hat{x}, \|\hat{x}-X\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y}\right]$

- $\mathcal{D}$ unknown → approximate it with a sample average + classification loss is non-continuous → use a smooth loss ⇒

$\min_\theta \frac{1}{N} \sum_{n=1}^N \max_{\hat{x}_n, \|x_n - \hat{x}_n\| \leq \varepsilon} \ell(y_n g_\theta(\hat{x}_n))$

1) $\forall x_n$, $\hat{x}_n^\star \approx \arg\max_{||x_n - \hat{x}_n| \leq \varepsilon} \ell(y_n g_\theta(\hat{x}_n))$
2) GD step w.r.t. θ using $\frac{1}{N} \sum_{n=1}^N \nabla_\theta \ell(y_n g_\theta(\hat{x}_n^\star))$

Advantages

- state-of-the-art approach for robust classification
- more interpretable gradients
- fully compatible with SGD

Disadvantages

- Increased computational time: proportional to the number of PGD steps
- Robustness-accuracy tradeoff: using too large ε leads to worse standard accuracy

Adversarial Example

$x \in \mathbb{R}^d, y \sim Bernoulli(\{-1, 1\}), Z_i \sim \mathcal{N}(0, 1)$

- Robust features: $x_1 = y + Z_1$
- Non-robust features: $x_i = y\sqrt{\frac{\log d}{d-1}} + Z_i$, $\forall i \in \{-1, 1\}$
- $d \to \infty \Rightarrow \uparrow$ adversarial risk and $\downarrow$ standard risk
- using the robust feature x_1:

MLE: $\arg\max_{\hat{y} \in \{\pm 1\}} p(\hat{y} \mid x_1) =$
$\arg\max_{\hat{y} \in \{\pm 1\}} \frac{p(x_1|\hat{y})p(\hat{y})}{p(x_1)} = \arg\max_{\hat{y} \in \{\pm 1\}} p(x_1 \mid \hat{y})$ assuming $p(y = 1) = p(y = -1)$

- Standard Risk: $\int_0^\infty \frac{1}{\sqrt{2\pi}} e^{-0.5(x+1)^2} dx \approx 0.16$ good but not perfect!
- using both robust and non-robust features:

MLE for all features $x_i = ya_i + Z_i$
$\arg\max_{\hat{y} \in \{\pm 1\}} p(\hat{y} \mid x)$
$= \arg\max_{\hat{y} \in \{\pm 1\}} \prod_{i=1}^d p(x_i \mid \hat{y})$
$= \arg\max_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d \log p(x_i \mid \hat{y})$
$= \arg\max_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d \log \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x_i - \hat{y}a_i)^2}$
$= \arg\min_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d (x_i - \hat{y}a_i)^2$
$= \arg\min_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d (x_i^2 - 2x_i\hat{y}a_i + \hat{y}^2 a_i^2)$
$= \arg\max_{\hat{y} \in \{\pm 1\}} \hat{y} \sum_{i=1}^d x_i a_i$
$\hat{y} \sum_{i=1}^d x_i a_i = \hat{y}y(\sum_{i=1}^d a_i^2) + \hat{y} \sum_{i=1}^d a_i Z_i = \hat{y}y(1 + \log(d)) + \hat{y}Z$ where $Z := \sum_{i=1}^d a_i Z_i \sim \mathcal{N}(0, 1 + \log d)$

Scaling by $1/(1 + \log d)$ the MLE results in: $y\hat{y} + \hat{y}Z$ with $Z \sim \mathcal{N}(0, 1/(1 + \log d))$
$d \to \infty, \hat{y}Z \to 0 \Rightarrow$ standard risk $R(f) \to 0$

- using the non-robust features improves standard risk!
- Adversarial risk:

The adversary can use tiny ℓ_∞ perturbations:
$\varepsilon = 2\sqrt{\frac{\log d}{d-1}}$ ($\to 0$ when) $d \to \infty$)
$\hat{x}_1 = \left(1 - 2\sqrt{\frac{\log d}{d-1}}\right) y + Z_1$, almost unaffected
$\hat{x}_i = -\sqrt{\frac{\log d}{d-1}} y + Z_i$, completely flipped
$R_\varepsilon(f) \approx 1 \Rightarrow$ tradeoff between accuracy and robustness.

Matrix Factorization

Given items (movies) $d = 1, 2, ..., D$ and users $n = 1, 2, ..., N$, we define X to be the $D \times N$ matrix containing all rating entries. That is, x_{dn} is the rating of n-th user for d-th item. Note that most ratings x_{dn} are missing, and our task is to predict them accurately.

Algorithm

$X \approx WZ^T$, $W \in \mathbb{R}^{D\times K}$, $Z \in \mathbb{R}^{N\times K}$ tall matrices $K << N, D$

$\min_{W,Z} \mathcal{L}(W,Z) := \frac{1}{2}\sum_{(d,n)\in\mathbb{Q}}[x_{dn} - (WZ^T)_{dn}]^2$

- We hope to "explain" each rating x_{dn} by a numerical representation of the corresponding item and user - in fact by the inner product of an item feature vector with the user feature vector.
- The set $\Omega \subseteq [D] \times [N]$ collects the indices of the observed ratings of the input matrix X.
- This cost is not jointly convex w.r.t. W and Z, nor identifiable as $(w^*, z^*) \Leftrightarrow (\beta w^*, \beta^{-1} z^*)$

Choosing K

- $\uparrow K \Rightarrow$ overfitting ($\Leftrightarrow \downarrow K \Rightarrow$ underfitting). For $K >> N, D \Rightarrow (W^*, {Z^*}^T) = (X, I) = (I, X)$

Regularization

$\frac{1}{2}\sum_{(d,n)\in\Omega}[x_{dn} - (WZ^T)_{dn}]^2 + \frac{\lambda_w}{2}||W||^2_{\text{Frob}} + \frac{\lambda_z}{2}||Z||^2_{\text{Frob}}$ $\lambda_w, \lambda_z \in \mathbb{R} > 0$

Stochastic Gradient Descent

$\mathcal{L} = \frac{1}{|\Omega|}\sum_{(d,n)\in\Omega} \underbrace{\frac{1}{2}[x_{dn} - (\mathbf{W}\mathbf{Z}^\mathsf{T})_{dn}]^2}_{f_{d,n}}$

For one fixed element (d, n) of the sum, we derive the gradient entry (d', k) for W:

$\frac{\partial}{\partial w_{d',k}} f_{d,n}(W,Z) \in \mathbb{R}^{D\times K} =$
$\begin{cases} -\left[x_{dn} - (\mathbf{W}\mathbf{Z}^T)_{dn}\right] z_{n,k} & \text{if } d' = d \\ 0 \text{ otherwise} \end{cases}$

$\frac{\partial}{\partial z_{n',k}} f_{d,n}(W,Z) \in \mathbb{R}^{N\times K} =$
$\begin{cases} -\left[x_{dn} - (\mathbf{W}\mathbf{Z}^T)_{dn}\right] w_{d,k} & \text{if } n' = n \\ 0 \text{ otherwise} \end{cases}$

- cost: $\Theta(K)$ which is cheap!

Alternating Least Squares

- No missing entries:
$\frac{1}{2}\sum_{d=1}^{D}\sum_{n=1}^{N}\left[x_{dn} - \left(W\mathbf{Z}^\mathsf{T}\right)_{dn}\right]^2$
$= \frac{1}{2}\|\mathbf{X} - \mathbf{W}\mathbf{Z}^\mathsf{T}\|^2_{Frob}$

- We first minimize w.r.t. Z for fixed W and then minimize W given Z (closed form solutions):
$Z^\mathsf{T} := (\mathsf{W}^\mathsf{T}\mathsf{W} + \lambda_z \mathsf{I}_K)^{-1}\mathsf{W}^\mathsf{T}\mathsf{X}$
$\mathbf{W}^\mathsf{T} := (\mathbf{Z}^\mathsf{T}\mathbf{Z} + \lambda_w \mathbf{I}_K)^{-1}\mathbf{Z}^\mathsf{T}\mathbf{X}^\mathsf{T}$
- Cost: need to invert a $K \times K$ matrix
- With missing entries: Can you derive the ALS updates for the more general setting, when only the ratings $(d,n) \in \Omega$ contribute to the cost, i.e.
$\frac{1}{2}\sum_{(d,n)\in\Omega}\left[x_{dn} - (\mathsf{W}\mathsf{Z}^\mathsf{T})_{dn}\right]^2$
Compute the gradient with respect to each group of variables, and set to zero.

Text Representation

-Finding numerical representations for words is fundamental for all machine learning methods dealing with text data.

-Goal: For each word, find mapping (embedding) $w_i \mapsto \mathbf{w}_i \in \mathbb{R}^K$

Co-Occurence Matrix

-A big corpus of un-labeled text can be represented as the co-occurrence counts. n_{ij} := #contexts where word w_i occurs together with word w_j.
- Needs definition of Context e.g. document, paragraph, sentence, window and Vocabulary $\mathcal{V} := \{w_1, \ldots, w_D\}$
- For words $w_d = 1, 2, \ldots, D$ and context words $w_n = 1, 2, \ldots, N$, the co-occurence counts n_{ij} form a very sparse $D \times N$ matrix.

Learning Word-Representations

- Find a factorization of the cooccurence matrix!
- Typically uses log of the actual counts, i.e. $x_{dn} := \log(n_{dn})$.
- Aim to find $\mathbf{W}, \mathbf{Z}$ s.t. $\mathbf{X} \approx \mathbf{W}\mathbf{Z}^\top$
$\min_{\mathbf{W},\mathbf{Z}} \mathcal{L}(\mathbf{W},\mathbf{Z}) :=$
$\frac{1}{2}\sum_{(d,n)\in\Omega} f_{dn}\left[x_{dn} - \left(\mathbf{W}\mathbf{Z}^\top\right)dn\right]^2$
where $\mathbf{W} \in \mathbb{R}^{D\times K}$, $\mathbf{Z} \in \mathbb{R}^{N\times K}$, $K \ll D, N$, $\Omega \subseteq [D] \times [N]$ indices of non-zeros of the count matrix $\mathbf{X}$, f_{dn} are weights to each entry.

GloVe

A variant of word2vec.
$f_{dn} := \min\{1, (n_{dn}/n_{\max})^\alpha\}$, $\alpha \in [0;1]$ (e.g. $\alpha = \frac{3}{4}$)

Note: Choosing K; K e.g. 50, 100, 500

Training

- Stochastic Gradient Descent (SGD) ($\Theta(K)$ per step $\rightarrow$ easily parralelizable)
- Alternating Least-Squares (ALS)

Skip-Gram Model

- Uses binary classification (logistic regression objective), to separate real word pairs (w_d, w_n) from fake word pairs. Same inner product score = matrix factorization.
- Given w_d, a context word w_n is:
real = appearing together in a context window of size 5
fake = any word $w_{n'}$ sampled randomly: Negative sampling (also: Noise Contrastive Estimation)

Learning Representations of Sentences & Documents

- Supervised: For a supervised task (e.g. predicting the emotion of a tweet), we can use matrix factorization or CNNs. - Unsupervised:
Adding or averaging (fixed, given) word vectors,
Training word vectors such that adding/averaging works well
Direct unsupervised training for sentences (appearing together with context sentences) instead of words

Fast Text

Matrix factorization to learn document/sentence representations (supervised).
Given a sentence $s_n = (w_1, w_2, \ldots, w_m)$, let $\mathbf{x}_n \in \mathbb{R}^{|\mathcal{V}|}$ be the bag-of-words representation of the sentence.

$$\min_{\mathbf{W},\mathbf{Z}} \mathcal{L}(\mathbf{W},\mathbf{Z}) := \sum_{s_n \text{ a sentence}} f\left(y_n \mathbf{W}\mathbf{Z}^\top \mathbf{x}_n\right)$$

where $\mathbf{W} \in \mathbb{R}^{1\times K}, \mathbf{Z} \in \mathbb{R}^{|\mathcal{V}|\times K}$ are the variables, and the vector $\mathbf{x}_n \in \mathbb{R}^{|\mathcal{V}|}$ represents our n-th training sentence.
Here f is a linear classifier loss function, and $y_n \in \{\pm 1\}$ is the classification label for sentence $\mathbf{x}_n$.

Language Models

Selfsupervised training:

- Can a model generate text? train classifier to predict the continuation (next word) of given text
- Multi-class: Use soft-max loss function with a large number of classes D = vocabulary size
- Binary classification: Predict if next word is real or fake (i.e. as in word2vec)
- Impressive recent progress using large models, such as transformers

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1 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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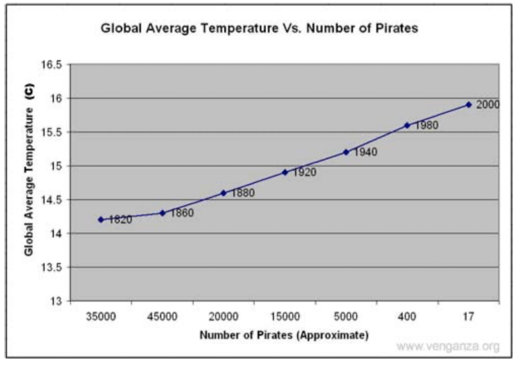

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