Statistical Computing

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Statistical Computing: What will we do?

Chapters

1. R in Action
2. Statistical Inference
3. Linear Models
4. Model Selection and Validation
5. Trees
6. Neural Nets

Remarks

- Chapters 3 to 6:
  Statistical ML in Action
- Two weeks per chapter
- Exercises at end of chapter notes

Neural Nets

Outline

- Understanding Neural Nets
- Practical Considerations
- Extended examples

Neural Nets

- Around since the 1950ies
- Underwent different development steps, e.g.
  - use of backpropagation (Werbos, 1974)
  - GPUs (2009, ImageNet 2012)
- Black Box
- TensorFlow/Keras, PyTorch

“Swiss Army Knife” among ML Algorithms

Can fit linear models

Fit data larger than RAM

Learn interactions
and non-linear terms

Non-linear
dimension reduction

Learn «online»

>1 Responses possible

Sequential and spatial
in- and output

Flexible and mixed
in- and output dimensions

Flexible loss functions

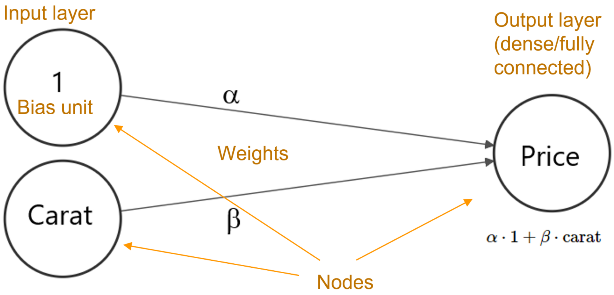
Understanding Neural Nets in three Steps

1. Linear regression as neural net
2. Hidden layers
3. Activation functions

Using diamonds data

Step 1: Linear Regression as Neural Net

- $\mathbb{E}(\text{price}) = \alpha + \beta \cdot \text{carat}$
- OLS
  $\hat{\alpha} \approx -2256$, $\hat{\beta} \approx 7756$
- Represented as neural network graph



Example

The Optimization Algorithm

Mini-batch gradient descent with backpropagation

Notation: Neural net f_β; its total loss on data D and loss function L:

$$Q(f_\beta, D) = \sum_{(y_i, \boldsymbol{x}_i) \in D} L(y_i, f_\beta(\boldsymbol{x}_i))$$

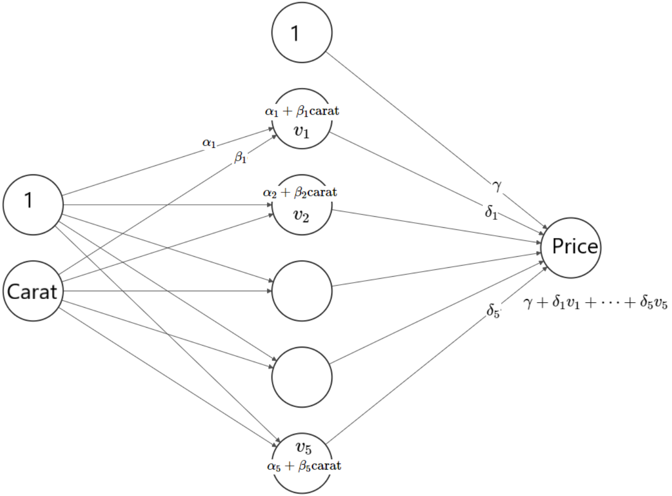
1. Init: Randomly initialize parameter vector β by $\hat{\beta}$
2. Forward: Calculate $Q(f_{\hat{\beta}}, D_{\text{batch}})$ on batch
3. Backprop: Modify $\hat{\beta}$ to improve $Q(f_{\hat{\beta}}, D_{\text{batch}})$
   3.1 Calculate partial derivatives $\nabla\hat{\beta} = \frac{\partial Q(f_\beta, D_{\text{batch}})}{\partial \beta} |_{\beta=\hat{\beta}}$ using backprop (=?)
   3.2 Gradient descent: Move slightly into right direction: $\hat{\beta} \leftarrow \hat{\beta} - \lambda \cdot \nabla\hat{\beta}$
4. Repeat Steps 2 and 3 until one epoch is over
5. Repeat Step 4 until some stopping criterion triggers

SGD? Local minima?

Step 2: Hidden Layers

- Add hidden layers for more parameters (= flexibility)
- Their nodes are latent/implicit variables
- Representational learning
- Encoding?
- Deep neural net?

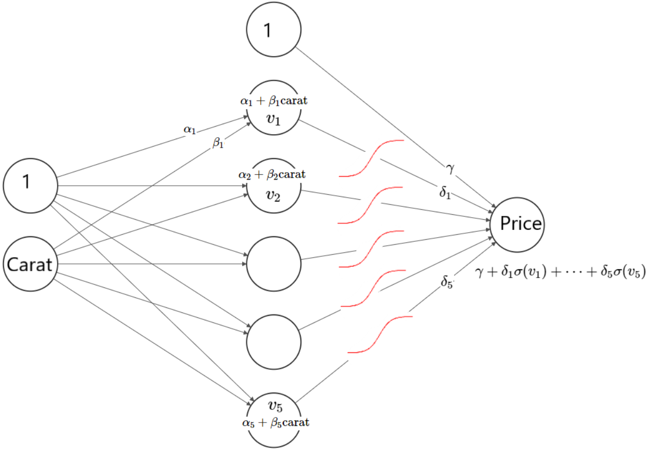
Example



Step 3: Activation Functions

Non-linear transformations σ of node values necessary!

- tanh: $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
- ReLU: $\sigma(x) = \max(0, x)$



Two purposes

- Imply interactions and non-linear terms
- Inverse link as in GLMs

Example

Practical Considerations

Validation and tuning of main parameters

Input standardization

Missing values

Categorical input

Callbacks

Types of layers

Interpretation

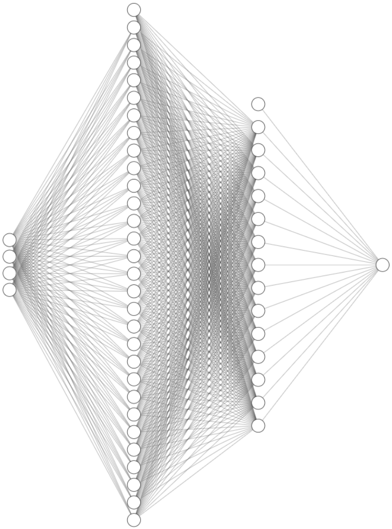
Optimizer

Overfitting and regularization

Choosing the architecture

Custom losses and evaluation metrics

Example: Diamonds



Excursion: Model-Agnostic Importance Measure

Permutation importance of feature $X^{(j)}$, data D, and performance measure S:

$$\mathrm{PVI}(j, D) = S(\hat{f}, D^{(j)}) - S(\hat{f}, D)$$

- $D^{(j)}$ is version of D with randomly permuted values in j-th feature column
- Read: How much S worsens after shuffling column j?
  The larger, the more important. If 0, feature is unimportant
- Computationally cheap $\rightarrow$ repeat m times
- Model is never refitted
- Training or test data?

Example

Embeddings

Represent unordered categorical X with K levels by $m << K$ numeric features

Embedding layer

- X integer encoded
- Dummy matrix $\tilde{X}$ with K columns
- Multiply $\tilde{X}$ with $(K \times m)$ matrix β
- Embedding matrix β estimated like other parameters
- Trick: $\tilde{X}\beta$ is calculated via index slicing from X and β
  $\rightarrow \tilde{X}$ is never materialized
- Think: $X_1 = j \rightarrow$ first row of $X\beta$ equals j-th row of β etc.

Example

Taxi trips

Excursion: Analysis Scheme X

$T(Y)$: quantity of interest

Steps

1. Calculate $T(Y)$ on the full data
2. Calculate $T(Y)$ stratified by covariates $X^{(j)} \rightarrow$ bivariate associations
3. Accompany Step 2 by ML model $\rightarrow$ multivariate associations
   - Study model performance
   - Study variable importance $\rightarrow$ sort results of Step 2
   - Study PDP (or similar) for each $X^{(j)}$ and compare with Step 2

Example

Comparison of ML Algorithms

Aspect	GLM	Neural Net	Decision Tree	Boosting	Random Forest	k-Nearest Neighbour
Scalable	😍	😍	😀	😀	😐	😟
Easy to tune	😐	😐	😐	😐	😀	😐
Flexible losses	😀	😍	😀	😀	😐	😐
Regularization	✔️	✔️	✔️	✔️	✔️	✔️
Case weights	✔️	✔️	✔️	✔️	✔️	✔️
Missing input allowed	😟	😟	✔️	✔️	😟	😟
Interpretation	😍	😐	😍	😐	😐	😐
Space on disk	😍	😍	😍	😀	😟	😟
Birth date (approx.)	1972 (Nelder & Wedderburn)	1974 Backprop (Werbos)	1984 (Breiman et al.)	1990 (Schapire)	2001 (Breiman)	1951 (Fix & Hodges)