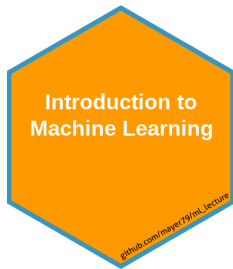


# Introduction to Machine Learning

Michael Mayer

October 2022



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## Intro

## Basics and Linear Models

- Basics

- Linear Regression

- Generalized Linear Models

## Model Selection and Validation

## Trees

- Decision Trees

- Random Forests

- Gradient Boosted Trees

## Neural Nets

## Final Words

*Data Science is 90% data preparation.  
This lecture is about the remaining 10%.*

## About Michael

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- ▶ Lecturer at ETH Zurich
- ▶ PhD in statistics
- ▶  $(M + C)^2$  Blog: <https://lorentzen.ch/>
- ▶ <https://github.com/mayer79>

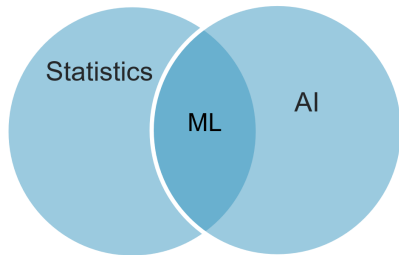
# What is Machine Learning (ML)?

Collection of statistical algorithms used to

1. predict things (supervised ML) or to
2. investigate data structure (unsupervised ML).

This lecture is on supervised ML

- ▶ Regression
- ▶ Classification



# Lecture Overview

## Chapters

1. Basics and Linear Models
2. Model Selection and Validation
3. Trees
4. Neural Nets

## Material

[https://github.com/mayer79/ml\\_lecture](https://github.com/mayer79/ml_lecture)

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# Before Modeling

- ▶ Organization of data?
- ▶ Data types?
- ▶ Descriptive analysis



## Structure of diamonds data

price	carat	color	cut	clarity
326	0.23	E	Ideal	SI2
326	0.21	E	Premium	SI1
327	0.23	E	Good	VS1
334	0.29	I	Premium	VS2
335	0.31	J	Good	SI2
336	0.24	J	Very Good	VVS2

## Example



# Statistical Models

## Setting

- ▶ Approximate **response variable**  $Y$  by function  $f$  of **covariates**  $X_1, \dots, X_m$

$$Y \approx f(X_1, \dots, X_m)$$

- ▶ Estimate unknown  $f$  from data by  $\hat{f}$ .
- ▶ Use  $\hat{f}$  for prediction and to investigate relationships.
- ▶ Postulate model equation  $\mathbb{E}(Y) = f(X_1, \dots, X_m)$   
(we are often interested in means).

## Remark

Other terms for response and covariates?

# Linear Regression

- ▶ Postulate

$$\mathbb{E}(Y) = f(X_1, \dots, X_m) = \beta_0 + \beta_1 X_1 + \dots + \beta_m X_m$$

- ▶ Interpretation of coefficients  $\beta_j$ ? Ceteris Paribus!
- ▶ Optimal  $\hat{\beta}_j$ ? Minimize sum of squared errors/residuals

$$\sum_{i=1}^n \underbrace{(y_i - \hat{y}_i)}_{\text{Residual}}^2$$

- ▶  $\hat{y} = \hat{f}(\dots)$  are predictions

## Example

Simple linear regression:  $\mathbb{E}(Y) = \alpha = \beta X$

# Aspects of Model Quality

## Predictive performance

- ▶  $\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$
- ▶ Root-MSE ( $\text{RMSE}$ )
- ▶ Relative performance:  
 $R^2 = 1 - \text{MSE}/\text{MSE}_0$
- ▶  $\text{MSE}_0 \rightarrow$  intercept-only model

## Validity of assumptions

- ▶ Model equation is correct
- ▶  $\text{Normal}$  linear model

$$Y = f(\dots) + \varepsilon \text{ with } \varepsilon \sim N(0, \sigma^2)$$

## Example

## Typical Problems

**Missing values**

**Outliers**

**Overfitting**

**Collinearity**

# Categorical Covariates

- ▶ One-Hot-Encoding
- ▶ Dummy coding
- ▶ Interpretation?

## Example of One-Hot-Encoding

color	D	E	F	G	H	I	J
E	0	1	0	0	0	0	0
E	0	1	0	0	0	0	0
E	0	1	0	0	0	0	0
I	0	0	0	0	0	1	0
J	0	0	0	0	0	0	1
J	0	0	0	0	0	0	1
I	0	0	0	0	0	1	0
H	0	0	0	0	1	0	0
E	0	1	0	0	0	0	0
H	0	0	0	0	1	0	0

Example

# Linear Regression is Flexible

1. Non-linear terms
2. Interactions
3. Transformations like logarithms

These elements are essential but tricky!

# Non-Linear Terms

## Deal with non-linear associations to $Y$ ?

→ invest more parameters

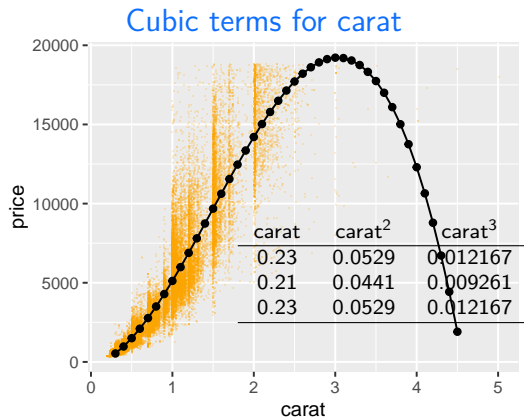
### 1. Polynomial terms

- ▶ E.g., cubic regression

$$\mathbb{E}(Y) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$

- ▶ Don't extrapolate!

### 2. Regression splines



Use systematic predictions

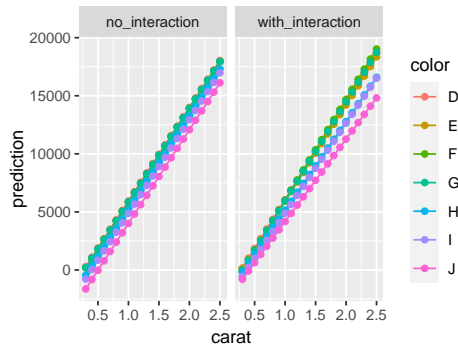
# Interactions

- ▶ Additivity of effects not always realistic

$$\mathbb{E}(Y) = \beta + \beta_1 X_1 + \cdots + \beta_m X_m$$

- ▶ Adding interaction terms brings necessary flexibility  $\rightarrow$  more parameters
- ▶ Interaction between features  $X$  and  $Z$ 
  - ▶ Multiplication (for categoricals?)
  - ▶ For categorical  $Z$ , effects of  $X$  are calculated by level of  $Z$
  - ▶ Like separate models per level of  $Z$

## Carat and color





# Transformations of Covariates

## Examples

- ▶ Dummy variables for categoricals
- ▶ Decorrelation
- ▶ Logarithms against outliers

Effects are interpreted for transformed covariates

# Logarithmic Covariates

- ▶  $\mathbb{E}(Y \mid X = x) = \alpha + \beta \log(x)$
- ▶ Properties of logarithm allow interpretation **for original covariate**
- ▶ A 1% increase in  $X$  is associated with an increase in  $\mathbb{E}(Y)$  of about  $\beta/100$
- ▶ Why?

$$\begin{aligned}\mathbb{E}(Y \mid 1.01x) - \mathbb{E}(Y \mid x) &= \alpha + \beta \log(1.01x) - \alpha - \beta \log(x) \\ &= \beta \log\left(\frac{1.01x}{x}\right) \\ &= \beta \log(1.01) \approx \beta/100\end{aligned}$$

## Example

# Logarithmic Responses

We see: log-transforming  $X$  allows to talk about relative effects in  $X$

Idea: log-transformed  $Y$  allows to talk about relative effects on  $Y$

Assume for a moment that

$$\mathbb{E}(\log(Y) \mid x) = \alpha + \beta x \implies \log(\mathbb{E}(Y \mid x)) = \alpha + \beta x$$

- ▶ Multiplicative model  $\mathbb{E}(Y \mid x) = e^{\alpha + \beta x}$
- ▶ Relative interpretation: “A one-point increase in  $X$  is associated with a relative increase in  $\mathbb{E}(Y)$  of  $100\%(e^{\beta} - 1) \approx 100\%\beta$ ”
- ▶ If also  $\log(X)$ ?

But assumption is wrong  $\rightarrow$  biased predictions for  $Y \rightarrow$  GLMs

Examples

## Example: Realistic Model for Diamond Prices

- ▶ Response:  $\log(\text{price})$
- ▶ Covariates:  $\log(\text{carat})$ , color, cut and clarity



## Exercise on Linear Regression

- ▶ Run last model without any logarithm
- ▶ Interpret the results
- ▶ Does model make sense from practical perspective?



# Generalized Linear Model (GLM)

(One) extension of linear regression

## Model equation

Two equivalent formulations

$$g(\mathbb{E}(Y)) = \beta_0 + \beta_1 X_1 + \cdots + \beta_m X_m$$

$$\mathbb{E}(Y) = g^{-1}(\beta_0 + \beta_1 X_1 + \cdots + \beta_m X_m)$$

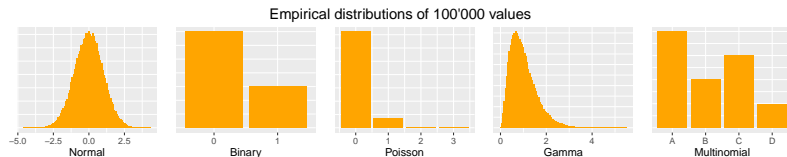
## Components

- ▶ Linear function/predictor
- ▶ Link function  $g$  to map  $\mathbb{E}(Y)$  to linear scale
- ▶ Distribution of  $Y$  conditional on covariates  $\rightarrow$  loss function (unit deviance)

# Typical GLMs

Regression	Distribution	Range of $Y$	Natural link	Unit deviance
Linear	Normal	$(-\infty, \infty)$	Identity	$(y - \hat{y})^2$
Logistic	Binary	$\{0, 1\}$	logit	$-2(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$
Poisson	Poisson	$[0, \infty)$	log	$2(y \log(y/\hat{y}) - (y - \hat{y}))$
Gamma	Gamma	$(0, \infty)$	$1/x$ (typical: log)	$2((y - \hat{y})/\hat{y} - \log(y/\hat{y}))$
Multinomial	Multinomial	$\{C_1, \dots, C_m\}$	mlogit	$-2 \sum_{j=1}^m 1(y = C_j) \log(\hat{y}_j)$

- Predictions?
- Log-Link?
- For binary  $Y$ :  
 $\mathbb{E}(Y) = P(Y = 1) = p$
- MSE  $\rightarrow$  Deviance
- Losses in ML?



# Why GLM, not Linear Regression?

Linearity assumption not always realistic

1. Binary  $Y$ :

Jump from 0.5 to 0.6 success probability less impressive than from 0.89 to 0.99

2. Count  $Y$ : Jump from  $\mathbb{E}(Y)$  of 2 to 3 less impressive than from 0.1 to 1.1.

3. Right-skewed  $Y$ :

Jump from 1 Mio to 1.1 Mio deemed larger than from 2 Mio to 2.1 Mio.

Logarithmic  $Y$  not possible in the first two cases

GLM solves problem by suitable link  $g$

Further advantages?



# Interpretation of Effects guided by Link

## Identity link

Like linear regression

## Log link

Like linear regression with log response

- ▶ Multiplicative model for response
- ▶ Now in mathematically sound way

## Logit link

- ▶ Additive model for  $\text{logit}(p)$
- ▶  $\text{logit}(p) = \log(\text{odds}(p)) = \log\left(\frac{p}{1-p}\right)$
- ▶ Remember:  $p = P(Y = 1) = \mathbb{E}(Y)$
- ▶ Multiplicative model for  $\text{odds}(p)$
- ▶ Coefficients  $e^{\beta} - 1 \approx 100\%\beta$  interpreted as odds ratios

## Examples with Insurance Claim Data

1. Poisson regression for claim counts
2. Binary logistic regression for claim (yes/no)

## Exercise on GLM

- ▶ Fit Gamma regression with log-link to explain diamond prices by  $\log(\text{carat})$ , color, cut and clarity.
- ▶ Compare the coefficients with corresponding linear regression for  $\log(\text{price})$ .
- ▶ Evaluate the relative prediction bias on USD scale.



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## Two Questions

- ▶ “How good is our model?”
- ▶ “Which model to choose among alternatives?”

### Problem and solution

- ▶ “Insample” performance is biased
- ▶ Overfitting should not be rewarded
- ▶ Use data splitting to get fair results

### Remarks

- ▶ Performance measure (evaluation metric) versus loss function?
- ▶ Confusion matrix?

## Excursion: $k$ -Nearest-Neighbour ( $k$ -NN)

- ▶ Alternative to linear model
- ▶ How does it work?
- ▶ Classification and Regression
- ▶ Standardization?

### Example

# Simple Validation

- ▶ Insample, 1-NN would win any comparison!?
- ▶ Split data into training and validation set, e.g., 80%/20%
- ▶ Use performance on validation set to make decisions (choose models, choose parameters like  $k$ )
- ▶ Measure amount of overfitting (= optimism)?

## Example

# Cross-Validation (CV)

Simple validation is neither economic nor robust, except for large data

## Algorithm

1. Split the data into  $k$  pieces  $D = \{D_1, \dots, D_k\}$  called “folds”. Typical  $k$ ?
2. Set aside one of the pieces ( $D_j$ ) for validation.
3. Fit model on all other pieces, i.e., on  $D \setminus D_j$ .
4. Calculate performance on the validation data  $D_j$ .
5. Repeat Steps 2–4 until each piece was used for validation once.
6. The average of the  $k$  model performances yields the **CV performance** of the model.

## Remarks

- ▶ How to choose and fit best/final model?
- ▶ What means «best»?
- ▶ Repeated CV?

## Example



# Hyperparameter Tuning

- ▶ Choosing  $k$  in  $k$ -NN is example of “hyperparameter tuning”
- ▶ Algorithms with more than 1 hyperparameter?
- ▶ Grid Search CV
- ▶ Randomized Search CV

# Test Data and Final Workflow

## Problematic consequence of model tuning?

- ▶ **Overfitting** on validation data or on CV!
- ▶ Performance of final model? → **Test data**

## Workflow A

1. Split data into train/valid/test, e.g., by ratios 70%/20%/10%.
2. Train different models on training data and assess their performance on the validation data. Choose best model, retrain on combination of training and validation data and call it “final model”.
3. Assess performance of final model on test data.

## Workflow B

1. Split data into train/test, e.g., by ratios 90%/10%.
2. Evaluate and tune different models by *k*-fold CV on the training data. Choose best model, retrain on full training data.
3. Assess performance of final model on test data.

## Example of Workflow B

When Test = Validation?

**Random splits**

**Grouped splits**

**Time-Series splits**

**Stratified splits**

## Exercises with Diamonds

1. As alternative to grouped splitting, deduplicate (why?) the diamonds data on "price" and all covariates and repeat the last example. Do the results change? Which results do you trust more?
2. Use CV to select the best polynomial degree of  $\log(\text{carat})$  in the Gamma GLM with log-link (with additional covariates color, cut, clarity). Evaluate on a test data.

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# Decision Trees

**Gradient  
Boosting**

**Random Forests**

# Decision Trees

- ▶ Simple
- ▶ Easy to interpret
- ▶ Decision trees are like wolves:  
Weak alone, strong together
- ▶ Around since 1984  
(Breiman, Friedman)



<https://images.pexels.com/photos/3732527/pexels-photo-3732527.jpeg>

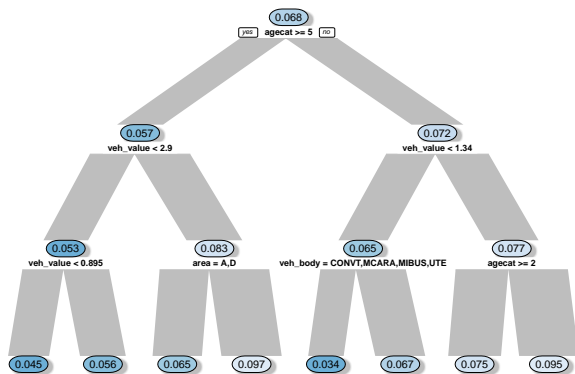
# How do Decision Trees Work?

## Algorithm

1. Split: find best “yes/no” question on best feature
2. Apply Step 1 recursively

## Notes

- ▶ “best” regarding average loss improvement
- ▶ Typical losses: squared error, log loss/cross-entropy/information or Gini
- ▶ Predictions?



The tree does a headstand

## Example



# Properties of Decision Trees

**Missing Values**  
**Interactions**

**Outliers**

**Categorical covariates**

**Greedy**

**Extrapolation**

Properties are inherited to groups/ensembles of decision trees

# Random Forests

- ▶ Combine many decision trees
- ▶ Perform very well
- ▶ Black Box
- ▶ Around since 2001 (Breiman)



<https://images.pexels.com/photos/1459534/pexels-photo-1459534.jpeg>

# How do Random Forests Work?

If we train 500 trees, how can we make sure they are different?

Idea: Introduce two sources of randomness

1. Each tree is trained on bootstrap sample.
2. Each split considers random selection of features only.

Predictions?

**Number of trees?**

**Diversification!**

**Out-of-Bag (OOB)**

**Insample  
performance**

**Parameter tuning**

Example

# Interpreting a Black Box is Important

Minimum interpretation of model?

1. Performance
2. Variable importance
3. Effects → e.g. partial dependence plots

Example

## Exercises on Random Forests

1. In our diamonds random forest, replace carat by  $\log(\text{carat})$ . Do the results change?
2. Fit a (probability) random forest on the claims data to predict claim probability by veh\_value, veh\_body, veh\_age, gender, area, and agecat.
  - ▶ Choose tree depth by OOB performance or CV.
  - ▶ Evaluate the model on an independent test dataset.
  - ▶ Interpret the results.

# Gradient Boosted Trees

- ▶ Combine many decision trees
- ▶ Perform very well
- ▶ Black Box
- ▶ Around since 2001 (Friedman)
- ▶ XGBoost, LightGBM, CatBoost

} Like random forests



<https://www.gormananalysis.com/blog/gradient-boosting-explained/>

# How does Gradient Boosting Work?

## Algorithm

1. Fit simple model (often a small decision tree).
2. Add another simple model to correct errors of first model.
3. Repeat Step 2 until stopping criterion triggers.

## Remarks

- ▶ Completely different from random forest.
- ▶ Predictions are found by combining predictions of all simple models (like random forest).
- ▶ Flexible regarding loss function.

Example XGBoost



# Parameter Tuning is Essential

1. Number of boosting rounds/trees  
→ find by early stopping (validation/CV)
2. Learning rate  
→ to get reasonable number of rounds
3. Regularization
  - ▶ Tree depth, number of leaves, loss penalties, etc.
  - ▶ → Grid/Randomized search and iterate

Why not one big  
grid search on  
all parameters?

Example XGBoost

# Exercises on Gradient Boosting

1. Study online documentation of XGBoost to make the last model monotonically increasing in carat. Check the resulting partial dependence plot.
2. Develop a strong XGBoost model on the claims data to predict claim probability by veh\_value, veh\_body, veh\_age, gender, area, and agecat.
  - ▶ Use `"binary:logistic"` as objective.
  - ▶ Use `"logloss"` as evaluation metric.
  - ▶ Use a clean CV/test strategy.
  - ▶ Interpret the results.

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# Neural Nets

- ▶ Around since the 1950ies
- ▶ Underwent different development steps, e.g.
  - ▶ use of backpropagation
  - ▶ GPUs
- ▶ Black Box
- ▶ TensorFlow/Keras, PyTorch

## “Swiss Army Knife” among ML Algorithms

**Can fit linear models**

**Learn interactions  
and non-linear terms**

**>1 Responses possible**

**Flexible and mixed  
in- and output dimensions**

**Fit data larger than RAM**

**Non-linear**      **Learn «online»**  
**dimension reduction**

**Sequential and spatial  
in- and output**

**Flexible loss functions**

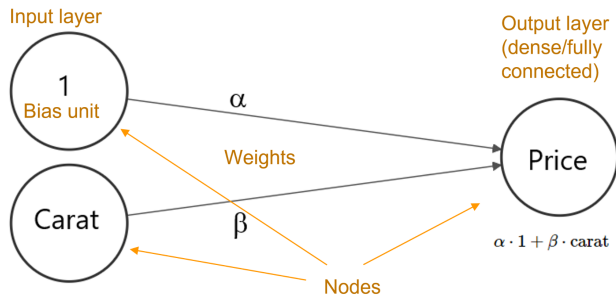
# Understanding Neural Nets in three Steps

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

Using **diamonds** data

## Step 1: Linear Regression as Neural Net

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



Example

# The Optimization Algorithm

## “Mini-batch gradient descent with backpropagation”

1. Init step: Randomly initiate parameters.
2. Forward step: Use parameters to calculate predictions of **batch**.
3. Backprop step: Evaluate **average loss** (e.g. MSE) of batch. Change parameters systematically to make it smaller.
4. Repeat Steps 2 and 3 until one **epoch** is over.
5. Repeat Step 4 until some stopping criterion triggers.

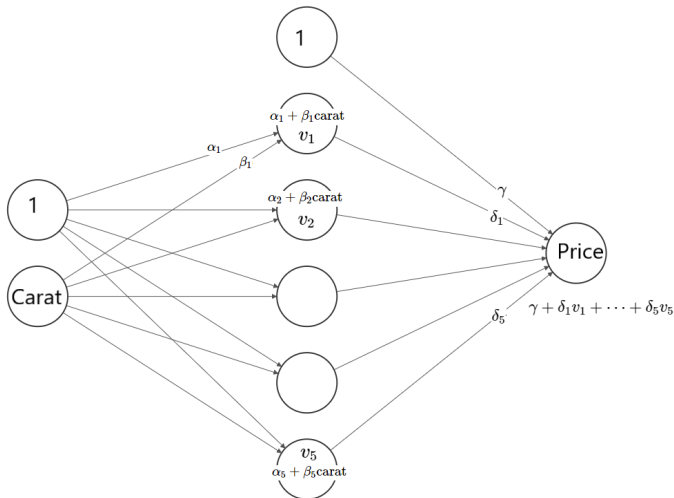
SGD? Gradients? Local minima?



## 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  $\sigma$  of node values necessary!

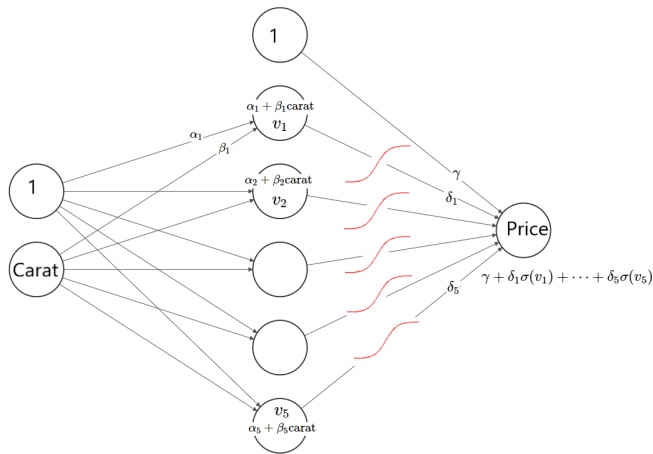
- ▶ tanh:  $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
- ▶ ReLU:  $\sigma(x) = \max(0, x)$



### Two purposes

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

### Example



# Practical Considerations

**Validation and tuning  
of main parameters**

**Callbacks**

**Overfitting and  
regularization**

**Input standardization**

**Missing values**

**Types of layers**

**Optimizer**

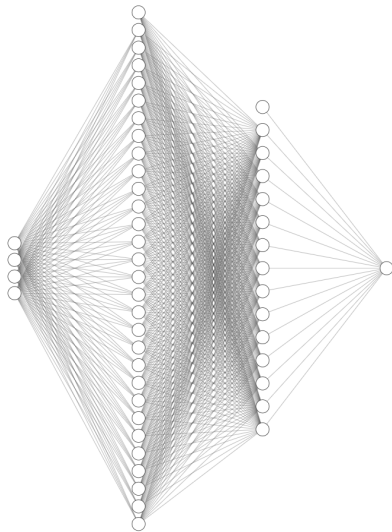
**Choosing the  
architecture**

**Categorical input**

**Interpretation**

**Custom losses and  
evaluation metrics**

## Example: diamonds



# Exercises on Neural Nets

1. Fit diamond prices by minimizing Gamma deviance with log-link (custom loss as in lecture notes; log-link means "exponential" output activation)
  - ▶ Tune model by simple validation.
  - ▶ Evaluate final model (for simplicity) on validation data.
  - ▶ Interpret final model.

Hints: Use smaller learning rate and replace "relu" by "tanh". Furthermore, the response is to be transformed from int to float.

2. Study either the optional claims data example in the lecture notes or build your own neural net, predicting claim yes/no.

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# 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)

## Analysis Scheme X

1. Take any property  $T(Y)$  of key interest (churn rate, claims frequency, loss ratio, etc.) and calculate its value on the full dataset.
2. Do a descriptive analysis of  $T(Y | X_j)$  for a couple of covariates to study the bivariate association between  $Y$  and each  $X_j$  separately.
3. Accompany Step 2 by ML model  $T(Y | X_1, \dots, X_p) \approx f(X_1, \dots, X_p)$ 
  - ▶ Check its performance.
  - ▶ Study variable importance and use it to sort the results of Step 2.
  - ▶ Study partial (or SHAP) dependence plots for each  $X_j$  and compare them with the associations from Step 2.

What did you learn from Step 3?