UNIVERSITY OF CAMBRIDGE

Advanced Data Science

Lecture 5 : Introduction to Statistical Learning

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The course so far

Access how to get and combine the data-sources for a potential problem

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Assess things to do with data before you have a question

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Access how to get and combine the data-sources for a potential problem

Assess things to do with data before you have a question

Address what you can do when you have data and a question to answer

Access

- ?

Assess

- Introduction to Probability (IA)
- Scientific Computing (IA)
- Cloud Computing (II)
- ....

Address

- ML and Real-world Data (IA)
- Data Science (IB)
- AI (IB)
- ML & Bayesian Inference (II)
- Deep NN (II)
- Randomised Algorithms (II)
- ....

Why?

Data centric thinking

You need to put Machine Learning in the context of data (and humans)
– Neil Lawrence

Reasons to use ML

- Tasks that are too hard to program
  - speech recognition
  - image understanding

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  - weather prediction
  - web search

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  - speech recognition
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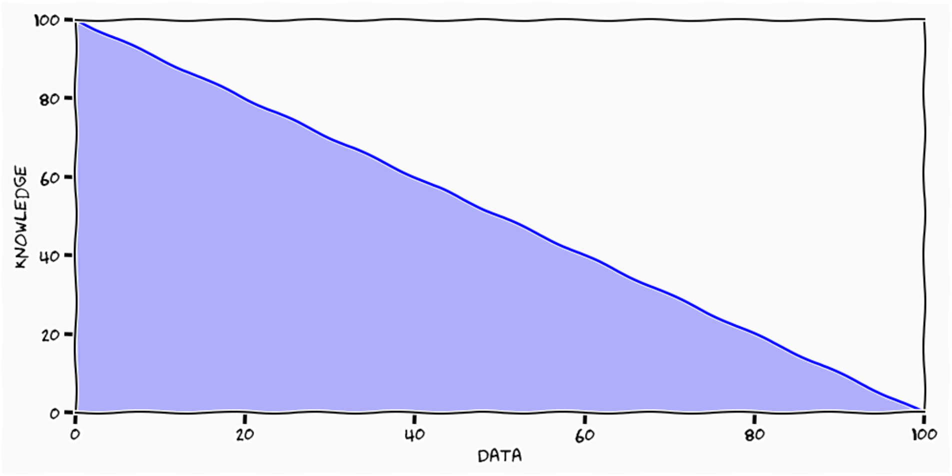
- Tasks beyond our capability
  - weather prediction
  - web search
- Machine Learning bridges the knowledge gap by data

Task of Statistical Learning



$$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta){\color{magenta}p(\theta)}}{p(\mathcal{D})}$$

- Inductive biases comes into the learning procedure

Machine Learning and Knowledge

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- *Most knowledge is introduced before we apply ML*

  access what data did I acquire?

  assess how did I prepare/treat the data?

Machine Learning and Knowledge

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  access what data did I acquire?

  assess how did I prepare/treat the data?
- The idea of the $80/20$

Today

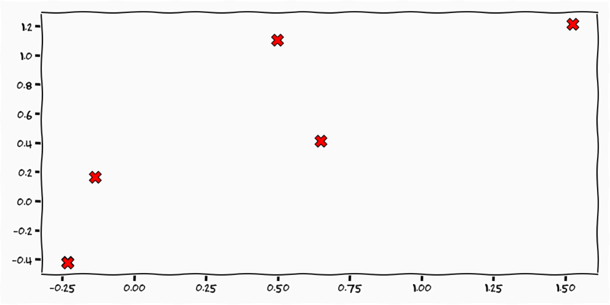
- what can machine learning actually do?
- what role does the "data scientist" play in the machine learning loop?
- put machine learning into context

Statistical Learning

Learning is the process of converting experience into expertise or knowledge.

– Sha Ben-David

Machine Learning Paradigms

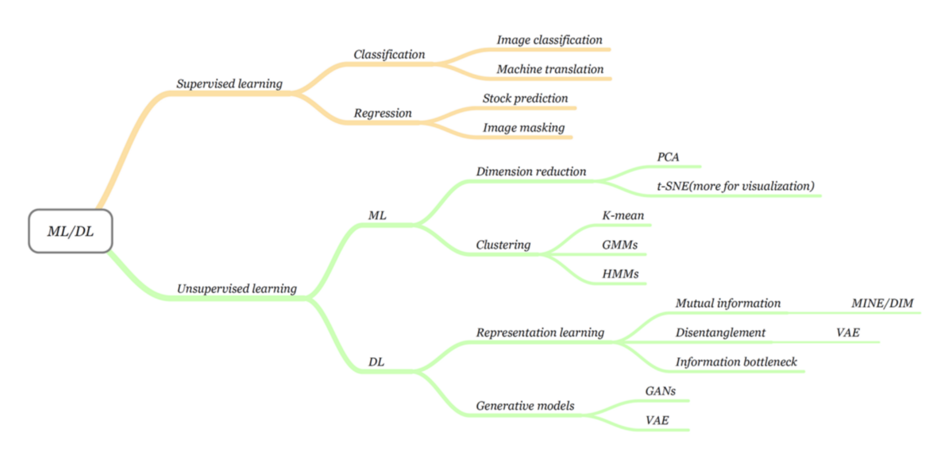


Supervised Learning $p(y \mid x)$

"Unsupervised" Learning $p(y)$

Reinforcement Learning $p(\pi, f \mid \mathcal{L})$

Machine Learning Methods



Formalism [Shalev-Shwartz et al., 2014]

Domain Set $\mathcal{X}$ the set of measurements/objects that we want to label (input)

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Label Set $\mathcal{Y}$ the set of outputs

Training Data $\mathcal{S}$ a finite sequence of pairs in $\mathcal{X} \times \mathcal{Y}$

Formalism [Shalev-Shwartz et al., 2014]

Data Distribution $\mathcal{D}$ probability distribution governing the measurements

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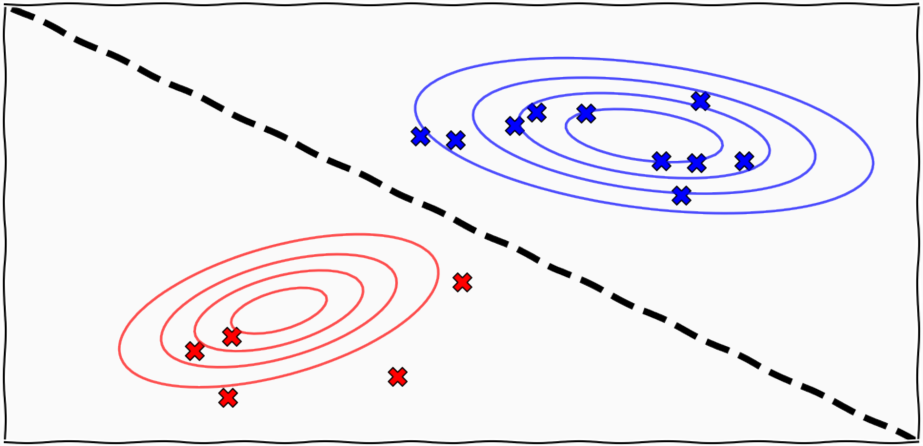
Data Generation $f : \mathcal{X} \to \mathcal{Y}$ the underlying generating process that we wish to recover

Prediction Rule $h : \mathcal{X} \to \mathcal{Y}$ what we wish to recover, the object that encodes the recovered knowledge

Classification



Measure of Success

$$L_{\mathcal{D},f}(h) := \mathcal{D}(\{x : h(x) \neq f(x)\})$$

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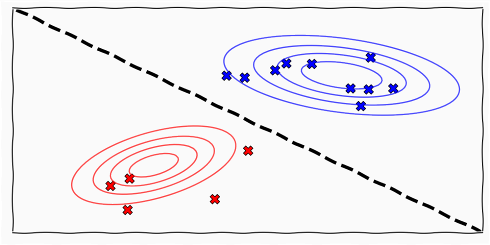
- we do not have access to f

Empirical Risk Minimisation

$$L_{\mathcal{S}}(h) := \frac{|\{i \in [m] : h(x_i) \neq y_i\}|}{m}$$

- We assume that $\mathcal{S} \sim \mathcal{D}$
- Empirical measure of risk

Overfitting

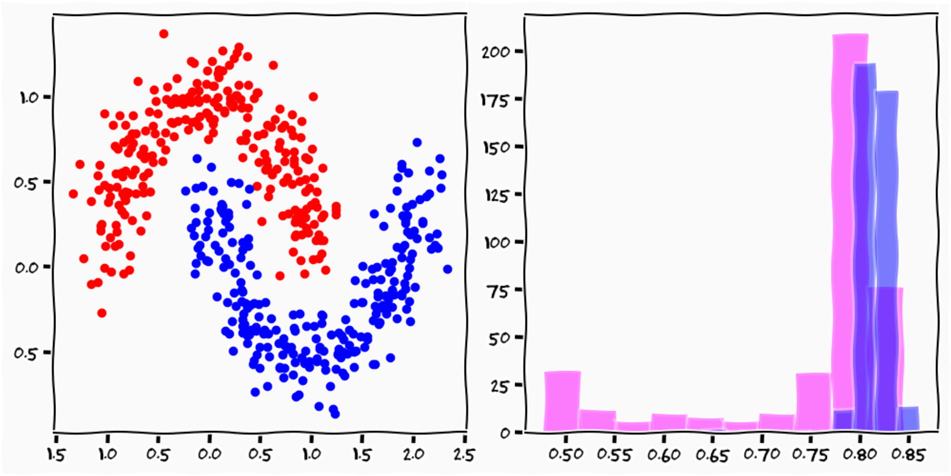


$$\mathcal{D} = \frac{1}{3}\mathcal{N}(\cdot,\cdot) + \frac{2}{3}\mathcal{N}(\cdot,\cdot)$$

$$h_{\mathcal{S}}(x) = \begin{cases} y_i & \text{if } \exists i \in [m] \text{s.t. } x_i = x \\ 0 & \text{otherwise} \end{cases}$$

- $L_{\mathcal{S}}(h_{\mathcal{S}}) = 0$ for all training data-sets
- if label 0 corresponds to red $L_{\mathcal{D}}(h_{\mathcal{S}}) = \frac{1}{3}$
- if label 0 corresponds to blue $L_{\mathcal{D}}(h_{\mathcal{S}}) = \frac{2}{3}$

True Risk is a Random Variable



Algorithm

$$L_{\mathcal{S}}(A(\mathcal{S})) := \frac{|\{i \in [m] : h(x_i) \neq y_i\}|}{m}$$

- We use an algorithm $A : \mathcal{S} \to h$ to find a hypothesis

Finite Hypothesis Classes

$$h_{\mathcal{S}} \in \underset{h \in \mathcal{H}}{\operatorname{argmin}}\, L_{\mathcal{S}}(h)$$

- We cannot parametrise all possible hypothesis

Statistical Learning Questions

m How much data do I need?

Statistical Learning Questions

m How much data do I need?

A How much does my solution depend on what I find?

Statistical Learning Questions

- m How much data do I need?
- A How much does my solution depend on what I find?
- H How does my solution depend on the hypothesis class I choose?

Probably Approximately Correct Learning

- We will assume the probability to get a non-representative sample to be δ

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- We have a threshold ϵ where we accept the hypothesis

$$L_{\mathcal{D},f}(h_{\mathcal{S}}) \leq \epsilon$$

Probably Approximately Correct Learning

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$$L_{\mathcal{D},f}(h_{\mathcal{S}}) \leq \epsilon$$

- We are looking for a *hypothesis* that will be probably (with confidence $(1-\delta)$) approximately (up to an error ϵ) correct.

Assumptions: I.I.D.

$$\mathcal{S} \sim \mathcal{D}^m$$

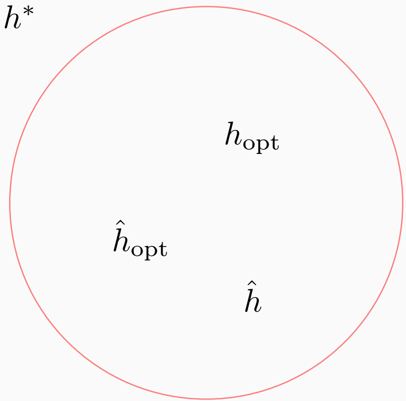
- each sample is *independent* from the other
- the *order* of samples does not effect the data distribution
- the sampling process does not effect the "world"

PAC Bounds [Shalev-Shwartz et al., 2014]

$$m \geq \frac{\log\left(\frac{|\mathcal{H}|}{\delta}\right)}{\epsilon}$$

- PAC learning allows us to provide bounds on the learning procedure
- How much data do we need?
- How large hypothesis class can we allow?

The Bias-Complexity Trade-off



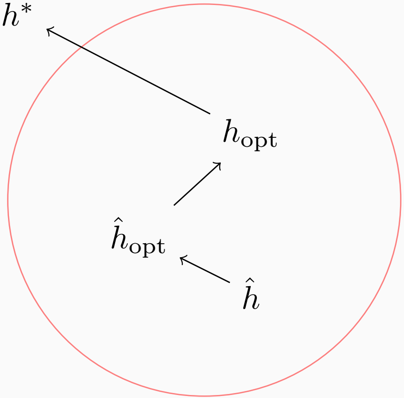
h^* the optimal predictor

$h_{\textbf{opt}}$ the optimal hypothesis

$\hat{h}_{\textbf{opt}}$ the optimal hypothesis on training data

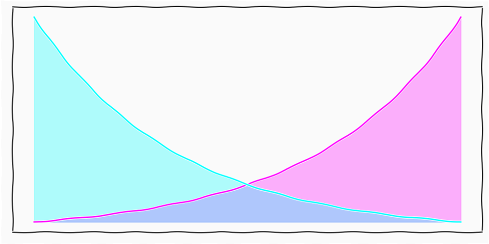
$\hat{h}$ the hypothesis found by learning algorithm

The Bias-Complexity Trade-off



$$
\begin{aligned}
&\epsilon(\hat{h}) - \epsilon(h^*) \\
&= \underbrace{\epsilon(h_{\mathsf{opt}}) - \epsilon(h^*)}_{\text{Approximation}} \\
&+ \underbrace{\epsilon(\hat{h}_{\mathsf{opt}}) - \epsilon(h_{\mathsf{opt}})}_{\text{Estimation}} \\
&+ \underbrace{\epsilon(\hat{h}) - \epsilon(\hat{h}_{\mathsf{opt}})}_{\text{Optimisation}}
\end{aligned}
$$

The Bias-Complexity Trade-off



High Complexity low bias (ϵ_{app} small), but high risk of overfitting (ϵ_{est} large)

Low Complexity high bias (ϵ_{app} large), low risk of overfitting (ϵ_{est} small)

Universal Learner

Theorem (The No-Free-Lunch Theorem)
Let A be any learning algorithm fo the task of binary classification with respect to $0-1$ loss over the domain $\mathcal{X}$. Let m be any number smaller than $\frac{|\mathcal{X}|}{2}$. Then there exists a distribution $\mathcal{D}(\{\mathcal{X} \times \{0,1\}\})$ such that,

- *There exists a function $f : \mathcal{X} \to \{0,1\}$ with $L_{\mathcal{D}}(f) = 0$*
- *With probability at least $\frac{1}{7}$ over the choice of $\mathcal{S} \sim \mathcal{D}^m$ we have $L_{\mathcal{D}}(A(S)) \geq \frac{1}{8}$*

The No-Free Lunch Theorem

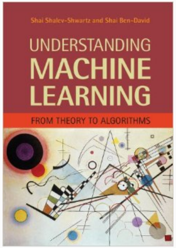
- There exists no universal learner
- For every learner there exist a task on which it fails
- Every algorithm that learns something useful does so by assumptions

The No-Free Lunch Theorem

- There exists no universal learner
- For every learner there exist a task on which it fails
- Every algorithm that learns something useful does so by assumptions
- There is no free lunch algorithm

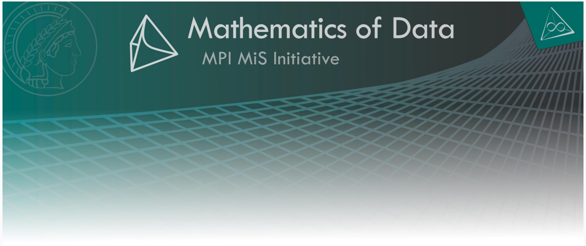
Statistical Learning Summary

- We can never have sufficient data
- We can never find a method that will guarantee to find the right solution
- We can never be certain about the true risk of our outcome



- Shai Shalev-Shwartz et al. (2014). *Understanding Machine Learning: From Theory to Algorithms*. New York, NY, USA: Cambridge University Press https://www.cs.huji.ac.il/~shais/UnderstandingMachineLearning/

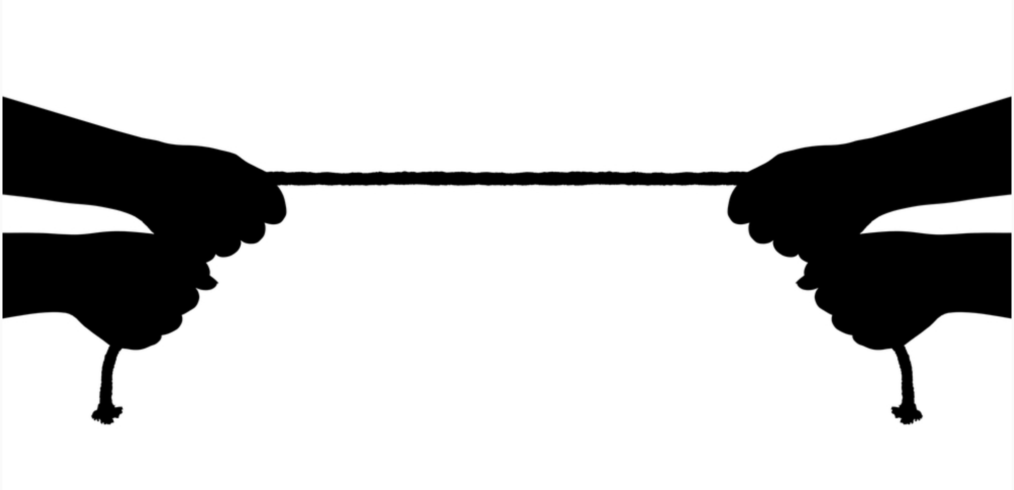
Statistical Learning Theory Further Reading



- O. Bousquet et al. (2004). "Introduction to Statistical Learning Theory". In: vol. Lecture Notes in Artificial Intelligence 3176. Heidelberg, Germany: Springer, pp. 169–207, http://www.econ.upf.edu/~lugosi/mlss_slt.pdf

Explicit vs. Tacit Knowledge

The Gap



The Gap

Access enormous inductive bias in what data to acquire

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Access enormous inductive bias in what data to acquire

Assess human bias in what questions will probably be asked

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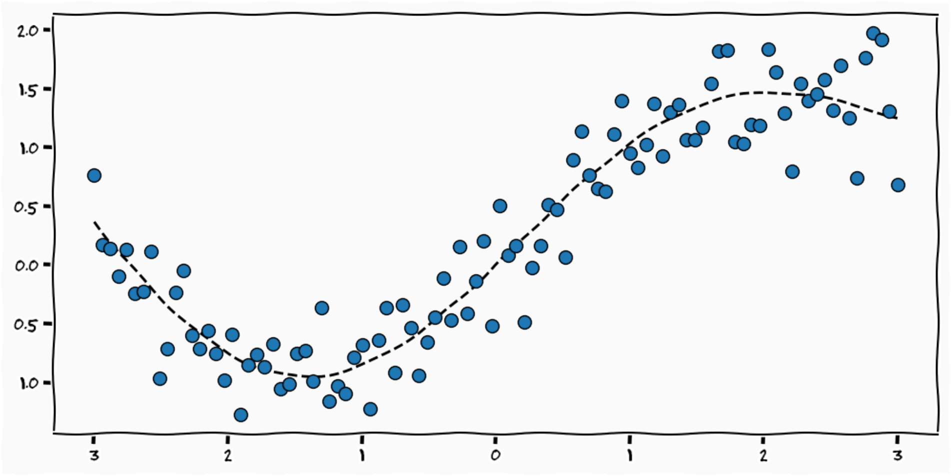
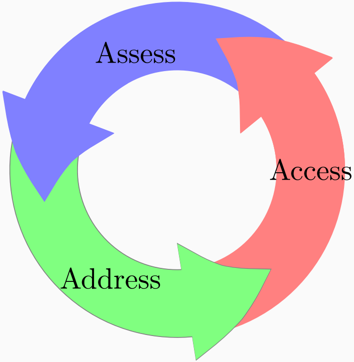
Assess human bias in what questions will probably be asked

Address "it is just curve fitting"

Curve Fitting is Really Fun



Requirements for Data Science



This part of the course

Today/Mon Generalised Linear Models

This part of the course

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Wen Unsupervised Learning

This part of the course

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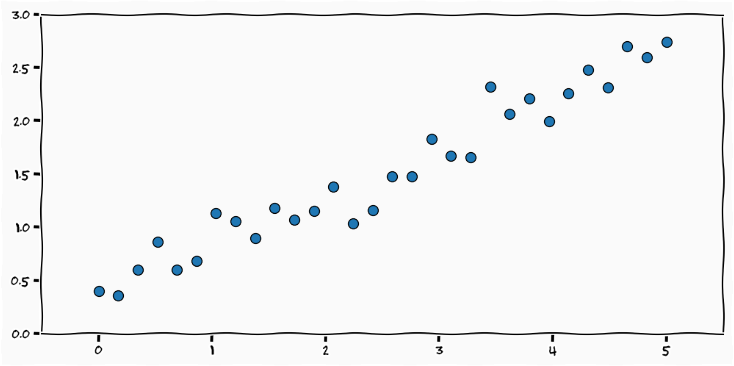
Fri Approximate Inference

Generalised Linear Models

Limited Hypothesis Classes

$$h \in \mathcal{H}$$

Formalism

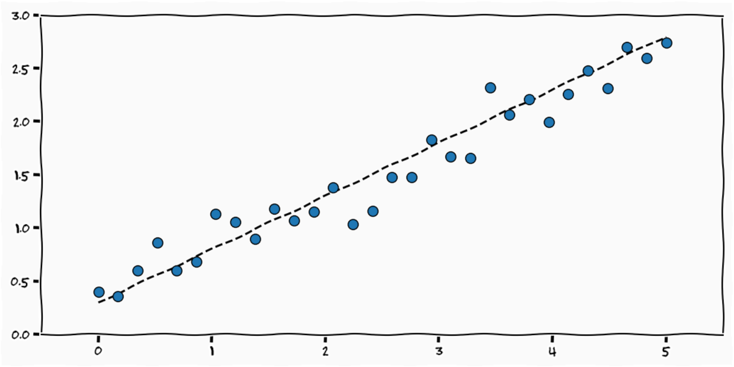


$\mathbf{x} \in \mathcal{X}$ explanatory variable

$y \in \mathcal{Y}$ response variable

Task *explain the response by the explanatory variables*

Linear Regression [Bishop, 2006]



$$y_i = \sum_{j=1}^{d} \beta_j x_{ij} + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \sigma^2).$$

Linear Regression Prediction

$$\mathbb{E}[y_i \mid \mathbf{x}_i] = \mathbb{E}\left[\sum_{j=1}^{d} \beta_j x_{ij} + \epsilon\right]$$

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&= \mathbb{E}\left[\sum_{j=1}^{d} \beta_j x_{ij}\right] + \mathbb{E}[\epsilon] \\
&= \sum_{j=1}^{d} \beta_j x_{ij} + 0.
\end{aligned}
$$

Linear Regression

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Linear Regression

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$$\hat{y}_i = \sum_{j=1}^{d} \beta_j x_{ij},$$

$$\hat{y}_i \sim \mathcal{N}(y_i, \sigma^2) = \mathcal{N}\left(\sum_{j=1}^{d} \beta_j x_{ij}, \sigma^2\right),$$

Generalised Linear Models [McCullagh et al., 1989]

$$g(\mathbb{E}[y_i \mid \mathbf{x}_i]) = \sum_{j=1}^{d} \beta_j x_{ij},$$

$g(\cdot)$ link function

$y \sim \mathcal{D}$ Exponential Dispersion Family

$\sum_{j=1}^{d} \beta_j x_{ij}$ Linear predictor

Generalised Linear Models [McCullagh et al., 1989]

$$\mathbb{E}[y_i \mid \mathbf{x}_i] = g^{-1}\Big(\sum_{j=1}^{d} \beta_j x_{ij}\Big),$$

- The inverse of the *link* maps the linear predictor to the first moment of the response
- Linear regression the link is identity

[1] https://towardsdatascience.com/glms-part-iii-deep-neural-networks-as-recursive-generalized-linear-URL

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- Looks an awful lot like a neural network[1]

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Exponential Dispersion Family [2]

$$f(y;\theta,\phi) = e^{\frac{\theta y - b(\theta)}{a(\phi)} + c(y,\phi)},$$

θ location parameter

ϕ scale parameter

[2] https://en.wikipedia.org/wiki/Exponential_dispersion_model

Gaussian

$$f(y;\mu,\sigma^2) = e^{\frac{\mu y - \frac{1}{2}\mu^2}{\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)}$$

- $\theta = \mu$
- $\phi = \sigma^2$
- $b(\theta) = \frac{1}{2}\mu^2$

- $a(\phi) = \sigma^2$
- $c(y,\phi) = \frac{y^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)$

Moments

$$\mathbb{E}[y \mid \mathbf{x}] = \frac{\partial}{\partial \theta} b(\theta)$$
$$\mathbb{V}[y \mid \mathbf{x}] = a(\phi) \frac{\partial^2}{\partial \theta^2} b(\theta).$$

- Through a consistent parametrisation we can generalise the moment calculations

Model	Response Variable	Link	Explanatory Variable
Linear Regression	Normal	Identity	Continuous
Logistic Regression	Binomial	Logit	Mixed
Poisson Regression	Poisson	Log	Mixed
ANOVA	Normal	Identity	Categorical
ANCOVA	Normal	Identity	Mixed
Loglinear	Poisson	Log	Categorical
Multinomial response	Multinomial	Generalized Logit	Mixed

Summary

Summary

- Brief introduction to statistical learning theory
- Take home
  - ML models and algorithms is only a small part of the story
  - we are doing a lot better than we should be
  - we are not sure what we are doing but it somehow works

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- Brief introduction to statistical learning theory
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  - ML models and algorithms is only a small part of the story
  - we are doing a lot better than we should be
  - we are not sure what we are doing but it somehow works
  - it is not explicit knowledge that pushes data-science forward, it is tacit and implicit

Summary

- Generalised Linear Models
  - "main" tool for statisticians
  - very well studied, excellent literature
  - linearity provides means of interpretability
  - excellent software packages `statsmodels`

The rest

Monday (22/11) Lecture: Generalised Linear Models

Tuesday (23/11) Lab: Generalised Linear Models

Wendesday (24/11) Lecture: Unsupervised Learning/Visualisation

Thursday (25/11) Tick: Generalised Linear Models

Friday (26/11) Lecture: Statistical Inference eof

References

- Bishop, Christopher M. (2006). *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Secaucus, NJ, USA: Springer-Verlag New York, Inc.
- Bousquet, O., S. Boucheron, and G. Lugosi (2004). "Introduction to Statistical Learning Theory". In: vol. Lecture Notes in Artificial Intelligence 3176. Heidelberg, Germany: Springer, pp. 169–207.
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- Shalev-Shwartz, Shai and Shai Ben-David (2014). *Understanding Machine Learning: From Theory to Algorithms*. New York, NY, USA: Cambridge University Press.