Introduction to Machine Learning

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DiscNet Summer School

June 2025

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Modules We Offer in Southampton

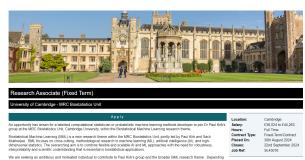
- Foundations of Machine Learning
- Machine Learning Technologies
- Advanced Machine Learning
- Differential Programming and Deep Learning
- Deep Learning Technologies
- Bayesian, Active & Reinforcement Learning
- Natural Language Processing
- Causal Reasoning and Machine Learning
- Computational Biology
- Computer Vision
- Computational Finance
- This week is a random sample from magenta

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Machine Learning: Good employment prospects!



Data scientist in quantitative finance Intellect UK Group Ltd. Hedge Fund 150 - 200K



Researcher in Biostatistics Medical Research Council, Cambridge Cancer Research 36 - 44K

Standard disclaimers apply!

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Foundations of Machine Learning ... draws from several disciplines

- Function approximation
- Linear algebra
 - Low rank approximation, Singular Value Decomposition
- Probability and Statistics
 - Multi-variate Gaussian, Information Theory, Bayes' Formula
- Optimization
- Software Engineering
- Parallel Computing
- Simulation, Experiment Design

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Machine Learning: Data-driven Modelling

Data $\{x_n, t_n\}_{n=1}^{N}$ $\{x_n\}_{n=1}^{N}$

Function Approximator $t = f(x, \theta) + v$

Parameter Estimation $E_0 = \sum_{n=1}^{N} \{|| \boldsymbol{t}_n - f(\boldsymbol{x}_n; \boldsymbol{\theta})||\}^2$

Prediction $\hat{\boldsymbol{t}}_{N+1} = f\left(\boldsymbol{x}_{N+1}, \, \hat{\boldsymbol{\theta}}\right)$

Regularization $E_1 = \sum_{n=1}^{N} \{||\boldsymbol{t}_n - f(\boldsymbol{x}_n)||\}^2 + r(||\boldsymbol{\theta}||)$

Modelling Uncertainty $p\left(\boldsymbol{\theta}|\left\{\boldsymbol{x}_{n},\boldsymbol{t}_{n}\right\}_{n=1}^{N}\right)$

Probabilistic Inference $\boldsymbol{E}\left[g\left(\boldsymbol{\theta}\right)\right] = \int g\left(\boldsymbol{\theta}\right) p\left(\boldsymbol{\theta}\right) d\boldsymbol{\theta} = \frac{1}{N_s} \sum_{n=1}^{N_s} g\left(\boldsymbol{\theta}^{(n)}\right)$

Sequential Estimation $\theta(n-1|n-1) \longrightarrow \theta(n|n-1) \longrightarrow \theta(n|n)$ Kalman & Particle Filters; Reinforcement Learning

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Good Books To study the fundamentals



T. Hastie, R. Tibshirani & J. Friedman Elements of Statistical Learning



C.M. Bishop

PRML: Pattern Recognition and Machine Learning



K. Murphy Proabilistic Machine Learning Probabilistic Machine Learning

Advanced Topics

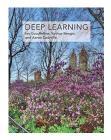
"There is nothing to be learnt from a professor, which is not to be met with in books" - David Hume (1711-1776)

(WikiPedia: "Hume had little respect for the professors of his time [...] He did not $\operatorname{graduate}$ ")

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More books...

For practical aspects of the subject...



I. Goodfellow et al. Deep Learning

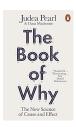


A. Geron Handson Machine Learning with Scikit-Learn

For some general, societally important, aspects of inference from data...



D. Spiegelhalter The Art of Statistics



J. Pearl The Book of Why



S.J. Gould Mismeasure of Man

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Machine Learning

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Machine Learning: Data-driven Modlling

Data

$$\{x_n, t_n\}_{n=1}^N \qquad \{x_n\}_{n=1}^N$$

$$\{\boldsymbol{x}_n\}_{n=1}^N$$

Function Approximator

$$t = f(x, \theta) + v$$

Parameter Estimation

$$E_0 = \sum_{n=1}^{N} \{ || \mathbf{t}_n - f(\mathbf{x}_n; \boldsymbol{\theta}) || \}^2$$

Prediction

$$\hat{\boldsymbol{t}}_{N+1} = f\left(\boldsymbol{x}_{N+1}, \, \hat{\boldsymbol{\theta}}\right)$$

Regularization

$$E_1 = \sum_{n=1}^{N} \{||\mathbf{t}_n - f(\mathbf{x}_n)||\}^2 + r(||\boldsymbol{\theta}||)$$

Modelling Uncertainty

$$\rho\left(\boldsymbol{\theta}|\left\{\boldsymbol{x}_{n},\boldsymbol{t}_{n}\right\}_{n=1}^{N}\right)$$

Probabilistic Inference

$$\boldsymbol{E}\left[g\left(\boldsymbol{\theta}\right)\right] = \int g\left(\boldsymbol{\theta}\right)p\left(\boldsymbol{\theta}\right)d\boldsymbol{\theta} = \frac{1}{N_{s}}\sum_{n=1}^{N_{s}}g\left(\boldsymbol{\theta}^{(n)}\right)$$

Sequential Estimation

$$\theta(n-1|n-1) \longrightarrow \theta(n|n-1) \longrightarrow \theta(n|n)$$

Kalman & Particle Filters; Reinforcement Learning

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Machine Learning Some Recent Challenges, Trends

- Function approximator: Shallow versus deep neural architectures
- Several tricks of parameter estimation of large (and deep) models
- Several tricks to induce generalization
- Automatic differentiation
- Problem formulation
 - Supervised & unsupervised versus Self-supervised learning
 - Human-in-the-loop Reinforcement Learning
 - Combining Mechanistic and Data-driven models e.g. Physics Informed Neural Networks
- Interesting problems in various domains.
- Large amounts of data (sometimes illegally acquired!)
- Large amounts of computing (only a few can afford!)

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Lab One: Multi-variate Gaussian

Univariate Gaussian

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2} \frac{(x-m)^2}{\sigma^2}\right\}$$

• Multivariate Gaussian $\mathbf{x} \in \mathcal{R}^D$

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{D/2}(\det \mathbf{\Sigma})^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \mathbf{m})^t \mathbf{\Sigma}^{-1}(\mathbf{x} - \mathbf{m}) \right\}$$

Mean m is a vector

Covariance, C, matrix: symmetric, positive definite!

$$oldsymbol{x} \sim \mathcal{N}(oldsymbol{m}, oldsymbol{\Sigma})$$
, $oldsymbol{y} = oldsymbol{A}oldsymbol{x} \implies oldsymbol{y} \sim \mathcal{N}(oldsymbol{A}oldsymbol{m}, oldsymbol{A}oldsymbol{\Sigma}oldsymbol{A}^{T})$

- Sampling from a given density
- Projections of data onto a subspace

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