Machine Learning 101

DESY Summer Program 2025 | July 31st 2025

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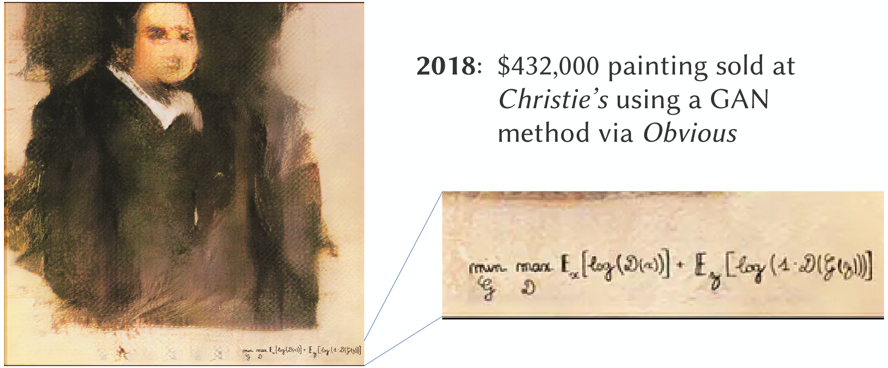
What is Machine Learning?



Portrait of Edmond de Belamy

2018: \$432,000 painting sold at *Christie's* using a GAN method via *Obvious*

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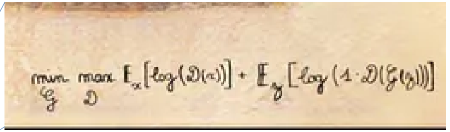

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Sparks the question of morality in the age of AI realism

X_1

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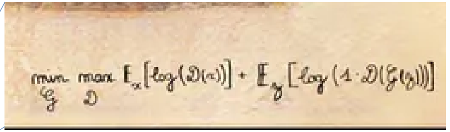

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2023: Tricking the world is not hard with such technology!


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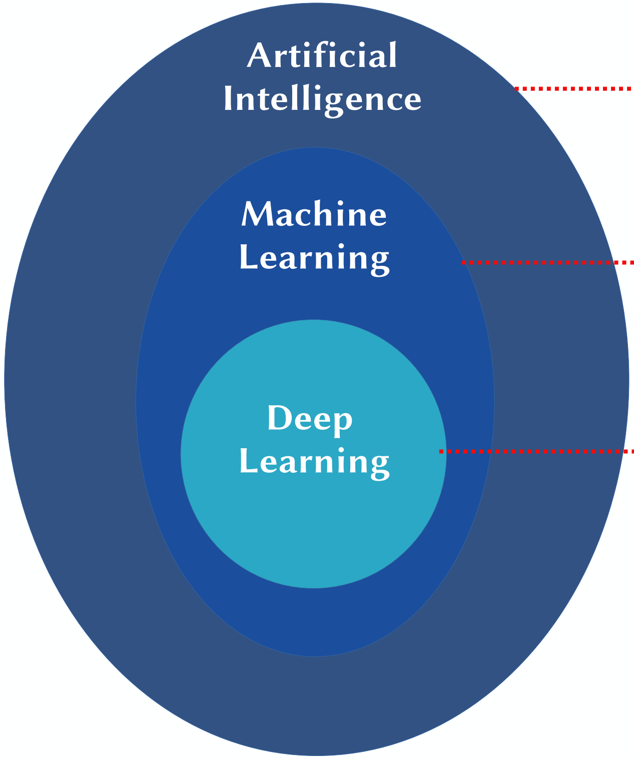
I thought I was immune to being fooled online. Then I saw the pope in a coat

Joel Golby

An encounter with an AI-generated image of his holiness has changed me: I now have sympathy for credulous baby boomers

'I thought wearing a really big coat and looking like a Metal Gear Solid 2 boss battle might have been part of his ongoing cool guy shtick. Lord, forgive me.' Photograph: Reddit

What is Machine Learning?



Artificial Intelligence:
Engineering behind intelligent machines and programs

Machine Learning:
Ability to learn without being explicitly programmed

Deep Learning:
Learning based on deep neural networks

What is Machine Learning?

'Giving computers the ability to learn without explicitly programming them'
- Arthur Samuel, 1959

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Paper: link

- *‘A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T , as measured by P , improves with experience E.’* - Mitchell 1997

[Mitchell 1997]: ISBN 0070428077

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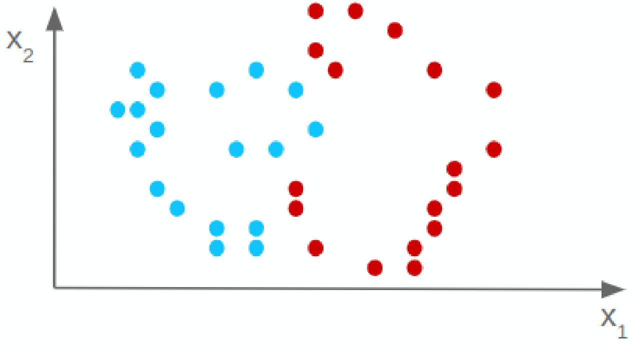
- **Experience (E):** The stimulus that drives learning, is the set of **examples** $\boldsymbol{x}$, or a **dataset** $\mathcal{D}$ of many examples $\mathbf{x} = \{x\}_N$:

  Supervised: The dataset examples have an associated label or target $\mathbf{y} = \{y\}_N$



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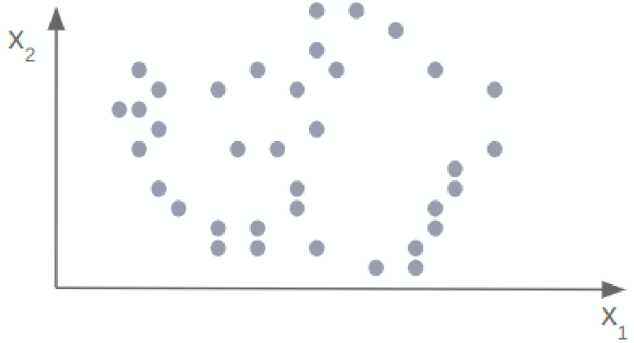
  Unsupervised: The dataset examples have **no** labels or targets



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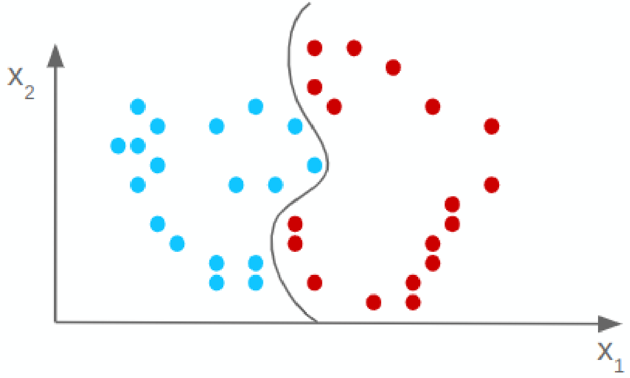
- **Task (T):** Given an **example** $\boldsymbol{x} \in \mathbb{R}^n$ the **model** $\boldsymbol{f}$ should learn a prediction $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$. E.g.

  Classification: Assign the example to a category $f : \mathbb{R}^n \to \{1,\ldots,k\}$

  Regression: Predict the value of a target $f : \mathbb{R}^n \to \mathbb{R}$



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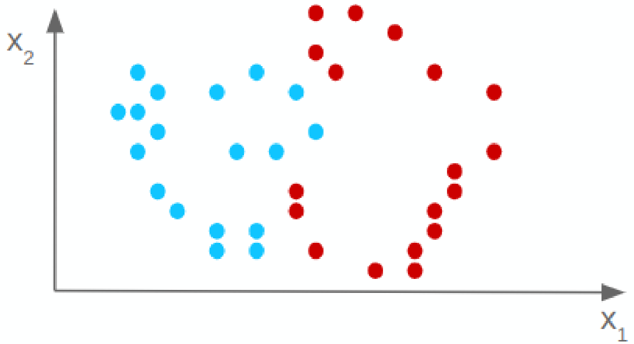
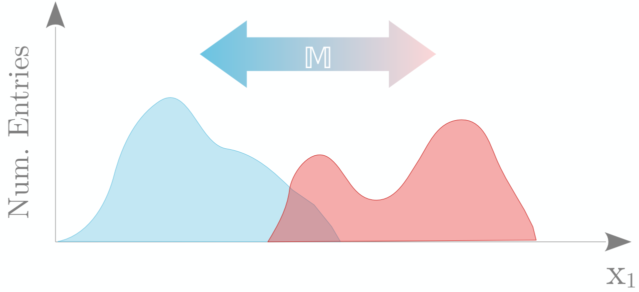


- **Performance (P):** Evaluate the performance of the **model *f***

  Measure Theory: Generalisation of geometric distances for a measureable space (Ω, F), such that for a measure $\mathbb{M} : F \rightarrow [0, +\infty]$



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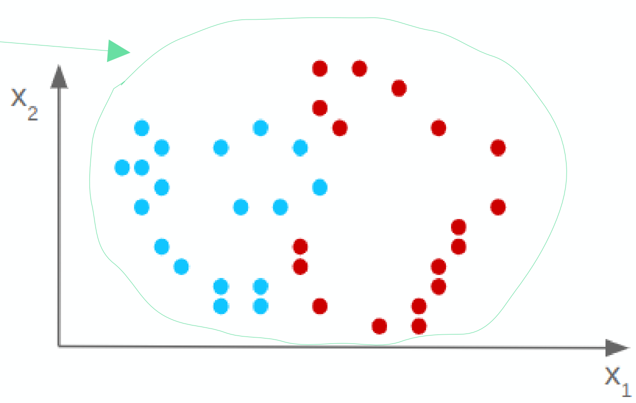
Basic Terminology - Day-to-day

- **Datasets:** The data from which the algorithm will need to learn from:

$$\mathcal{D} = \{ \{x_i , y_i\} \in \mathbb{R}^X \times \mathbb{R}^Y \}_N$$



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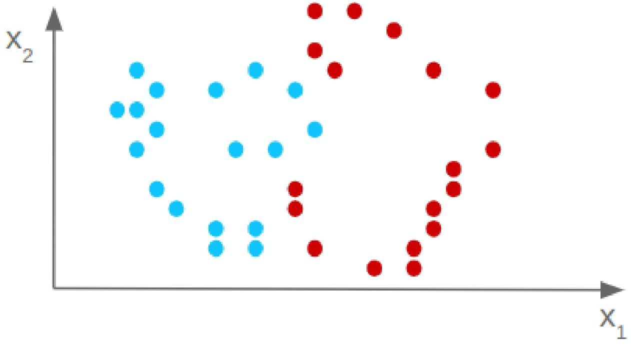
- **Features:** Each dimension of the example x, or input space $\mathbb{R}^X$, which represents some *feature* such as pixel color, particle energy, etc...:

$$x \in \mathbb{R}^X$$

$\mathbb{R}^2$



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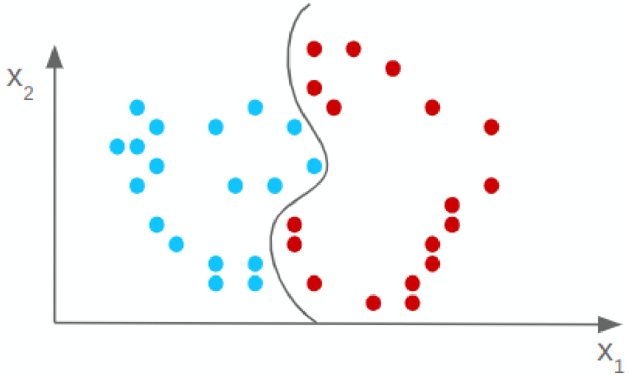
$$x \in \mathbb{R}^X$$

- **Algorithms:** The process in which the model f defined by a parameter set Φ is optimised according to some **objective function**:

$$\Phi^* = \arg\min_{\Phi} [\ f\ ]$$



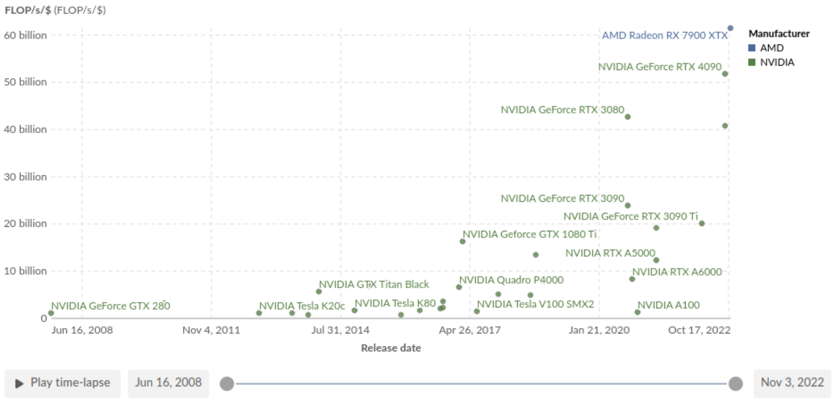
Is ML useful?

AI/ML Summer

- **The boom in ML/AI has been primarily the result of:**

  Datasets: The vast amount of data from images curated by ImageNet to Protein Data Bank (PDB)

  Processing Power: The computational power of CPU/GPUs and now emerging accelerator platforms such as TPUs etc…



- **At a secondary level it is also the result of:**

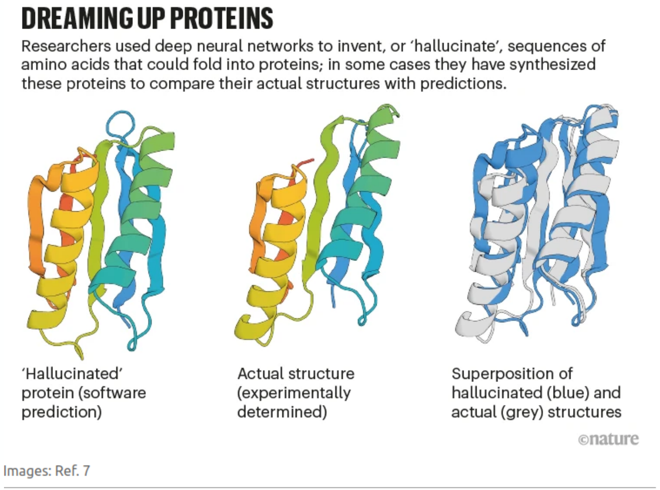
  Open-source Libraries: PyTorch (Meta), Tensorflow + JAX (Google), etc…

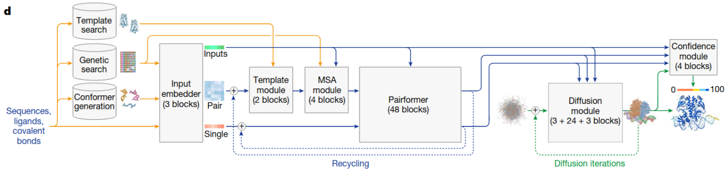
  High—Level Interpretable Languages: Julia, Python, etc…

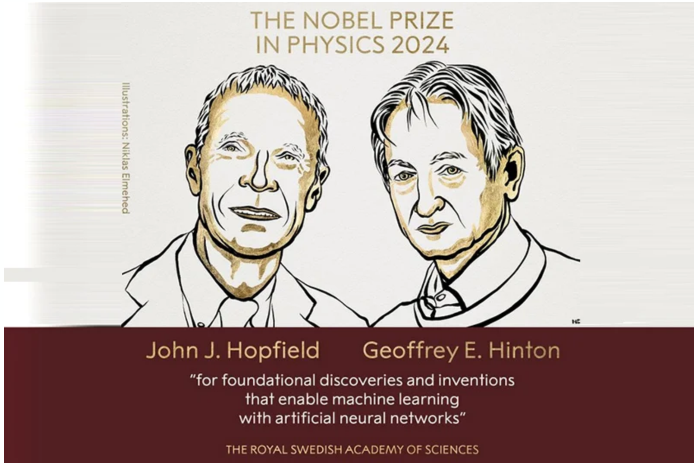
AI/ML Summer

- **Bio-molecular research:**

  AlphaFold1.0 → 3.0 has lead to substantial advancements in predicting protein structures:

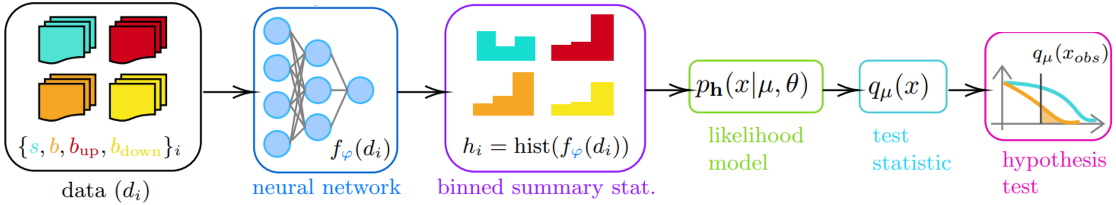






High Energy Physics – ML Developments

→ Checkout the HEP Machine Learning Living Review



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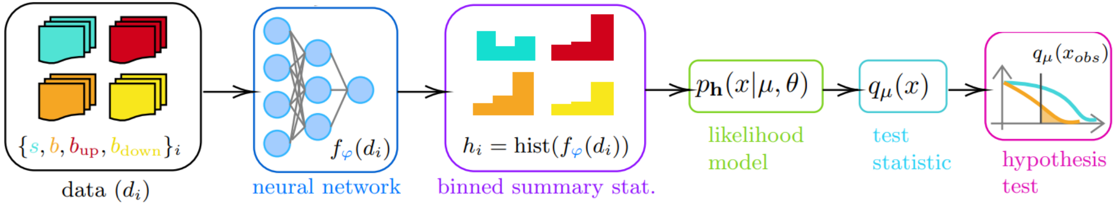
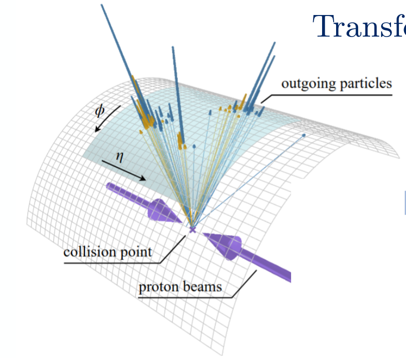
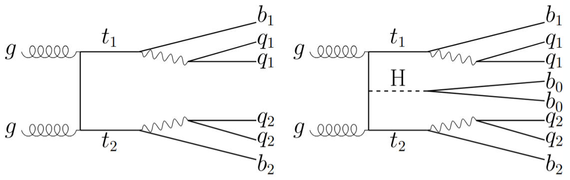


SPANet Transformer - arXiv:2106.03898

Transformer model using scaled dot-product equivariant properties for top-jet reconstruction





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	N_{jets}	Event Fraction	SPA-NET Efficiency Event	SPA-NET Efficiency Top Quark	χ^2 Efficiency Event	χ^2 Efficiency Top Quark
All Events	== 6	0.245	0.643	0.696	0.424	0.484
	== 7	0.282	0.601	0.667	0.389	0.460
	≥ 8	0.320	0.528	0.613	0.309	0.384
	Inclusive	**0.848**	**0.586**	**0.653**	**0.392**	**0.457**
Complete Events	== 6	0.074	0.803	0.837	0.593	0.643
	== 7	0.105	0.667	0.754	0.413	0.530
	≥ 8	0.145	0.521	0.662	0.253	0.410
	Inclusive	**0.325**	**0.633**	**0.732**	**0.456**	**0.552**

ttH

	N_{jets}	Event Fraction	SPA-NET Efficiency Event	SPA-NET Efficiency Higgs	SPA-NET Efficiency Top	χ^2 Efficiency Event	χ^2 Efficiency Higgs	χ^2 Efficiency Top
All Events	== 8	0.261	0.370	0.497	0.540	0.044	0.151	0.053
	== 9	0.313	0.343	0.492	0.514	0.038	0.146	0.066
	≥ 10	0.313	0.294	0.472	0.473	0.030	0.135	0.072
	Inclusive	**0.972**	**0.330**	**0.485**	**0.502**	**0.039**	**0.146**	**0.062**
Complete Events	== 8	0.042	0.532	0.657	0.663	0.016	0.151	0.063
	== 9	0.070	0.422	0.601	0.596	0.013	0.146	0.076
	≥ 10	0.115	0.306	0.545	0.523	0.008	0.134	0.080
	Inclusive	**0.228**	**0.383**	**0.583**	**0.572**	**0.012**	**0.144**	**0.073**

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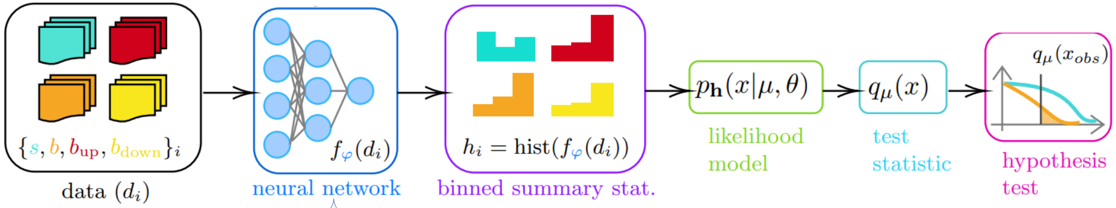
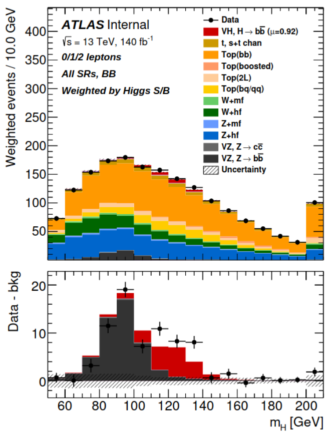
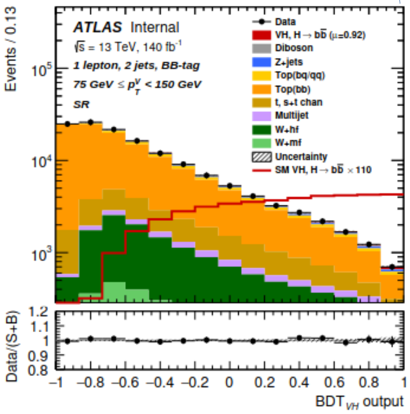


Typical signal classification in data analyses, e.g. Higgs discovery:

Analysis	Years of data collection	Sensitivity without machine learning	Sensitivity with machine learning	Ratio of P values	Additional data required
CMS[24] $H \to \gamma\gamma$	2011–2012	2.2σ, $P = 0.014$	2.7σ, $P = 0.0035$	4.0	51%
ATLAS[43] $H \to \tau^+\tau^-$	2011–2012	2.5σ, $P = 0.0062$	3.4σ, $P = 0.00034$	18	85%
ATLAS[99] $VH \to bb$	2011–2012	1.9σ, $P = 0.029$	2.5σ, $P = 0.0062$	4.7	73%
ATLAS[41] $VH \to bb$	2015–2016	2.8σ, $P = 0.0026$	3.0σ, $P = 0.00135$	1.9	15%
CMS[100] $VH \to bb$	2011–2012	1.4σ, $P = 0.081$	2.1σ, $P = 0.018$	4.5	125%

Source: A. Radovic et al., Nature 560(2018) no. 7716,41





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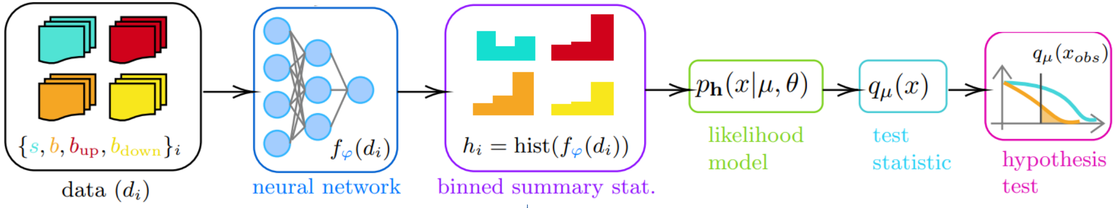
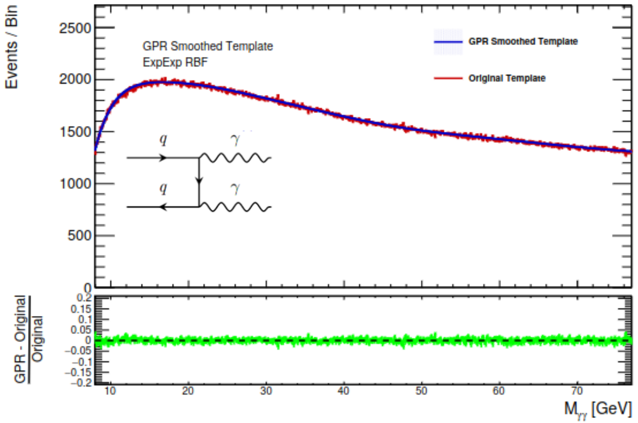


Background Estimation by smoothing data-driven backgrounds using gaussian processes for H→γγ

Source: CDS-2791079



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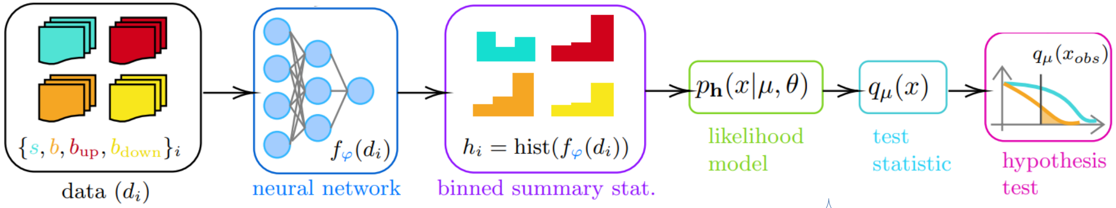
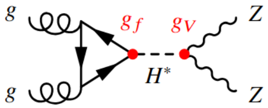
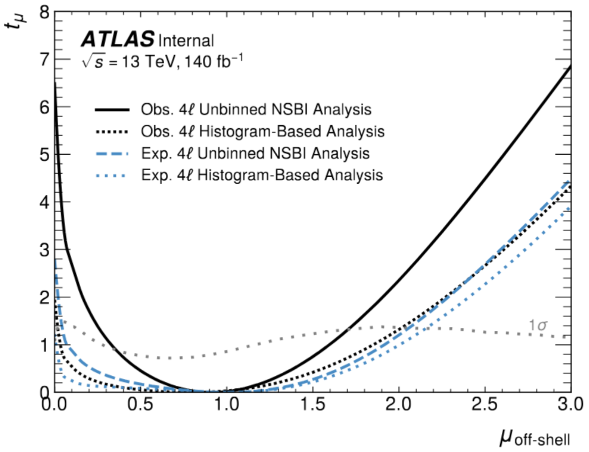


New likelihood inferencing paradigm:

H→ZZ off-shell analysis using unbinned likelihood ratios from neural networks

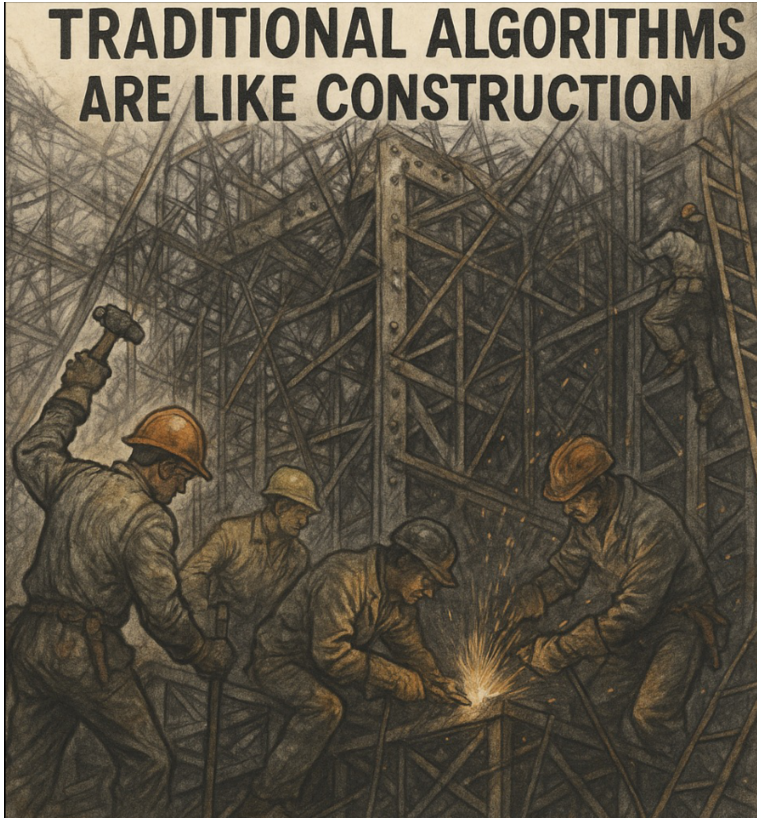




Source: ATL-COM-PHYS-2024-24

Learning Law

Machine Learning versus Algorithm Development



Learning Law

- **Four key parts** to the 'Machine Learning' process:

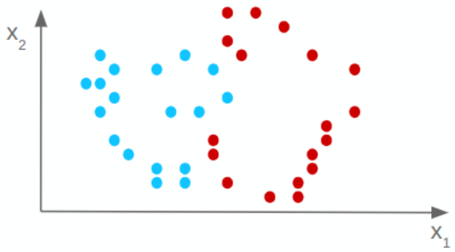
Dataset:

Supervised:

$$\mathcal{D} = \{ \{x_i , y_i\} \in \mathbb{R}^X \times \mathbb{R}^Y \}_N$$

Unsupervised:

$$\mathcal{D} = \{ \{x_i\} \in \mathbb{R}^X \}_N$$



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Model f:

E.g. Neural network with parameters Φ

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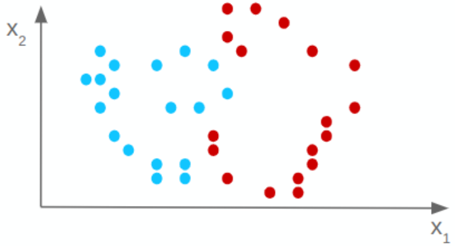

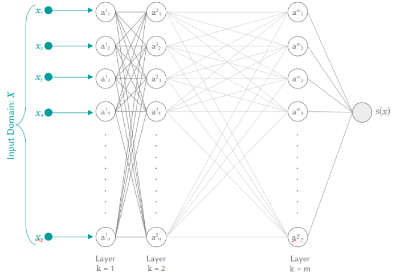

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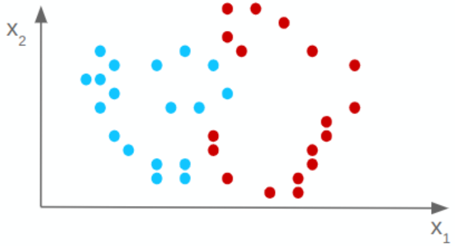
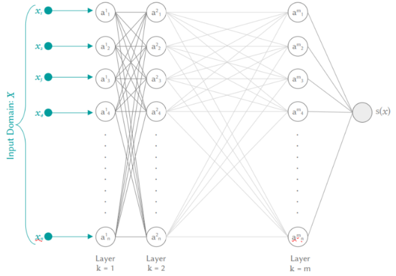
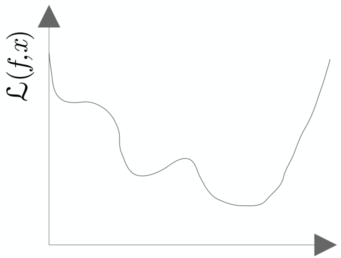
Unsupervised:
$\mathcal{D} = \{ \{x_i\} \in \mathbb{R}^X \}_N$

Loss/Cost Function
$\mathcal{L}(f,x)$:
Function for calculating agreement between prediction of model and implicit data distribution





$$\mathcal{D}_{\mathrm{KL}}(P||Q) = \mathbb{E}_{x\sim P}\left[\ln\left(P(x)\right) - \ln\left(Q(x)\right)\right]$$



Learning Law - Recipe

- **Four key parts** to the ‘Machine Learning’ process:

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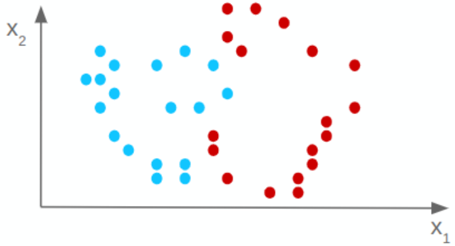
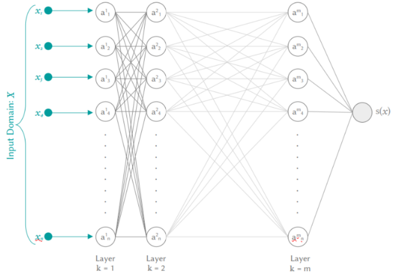
Unsupervised:
$\mathcal{D} = \{\ \{x_i\} \in \mathbb{R}^X\ \}_N$

Model f:
E.g. Neural network with parameters Φ

Loss/Cost Function $\mathcal{L}(f,x)$:
Function for calculating agreement between prediction of model and implicit data distribution

Optimise parameters Φ:
Optimisation algorithm





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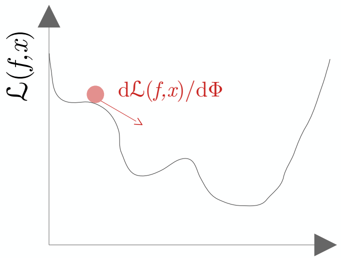


Brief Statistics Review

Frequentist Statistics

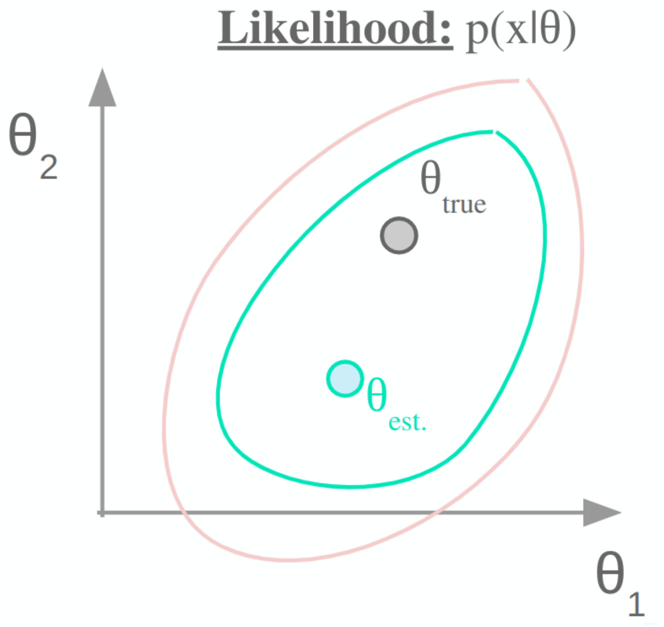
- **Probability** is attributed only to the data **x,** meaning probability of outcomes is obtained by repeatable experiments:

$$P(\mathbf{x} = x) = \lim_{n \to \infty} \frac{n_x}{N}$$

- **Conditional probability**, the probability of an outcome **(x**$=x$**)** conditioned on the occurance of another random process **(y**$=y$**):**

$$P(\mathbf{x} = x | \mathbf{y} = y) = \frac{P(\mathbf{x} = x, \mathbf{y} = y)}{P(\mathbf{x} = x)}$$

- **Important** to note that frequentist statistics assumes that the data is drawn from p(**x**$=x$ | θ), with a set of parameters that characterise the underlying true distribution θ.



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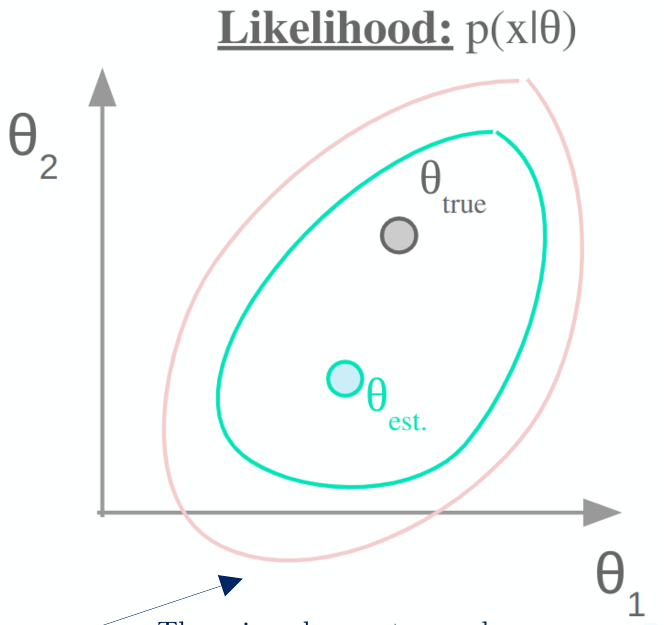
$$P(\mathbf{x} = x | \mathbf{y} = y) = \frac{P(\mathbf{x} = x, \mathbf{y} = y)}{P(\mathbf{x} = x)}$$

- **Important** to note that frequentist statistics assumes that the data is drawn from $p(\mathbf{x}{=}x \mid \theta)$, with a set of parameters that characterise the underlying true distribution θ.



There is only one true value of θ_{true}. The goal is to estimate it ~ $\theta_{est.}$

Bayesian Statistics

- **Probability** is a degree of belief meaning that the observed data **x,** is not necessarily defined by repeatability:

$$P(H|\mathbf{x}=x) = \frac{P(\mathbf{x}=x|H)P(H)}{\underbrace{\int P(\mathbf{x}=x|H)P(H)dH}_{\text{Normalise over all possible hypotheses} \sim \text{marginal probability}}}$$

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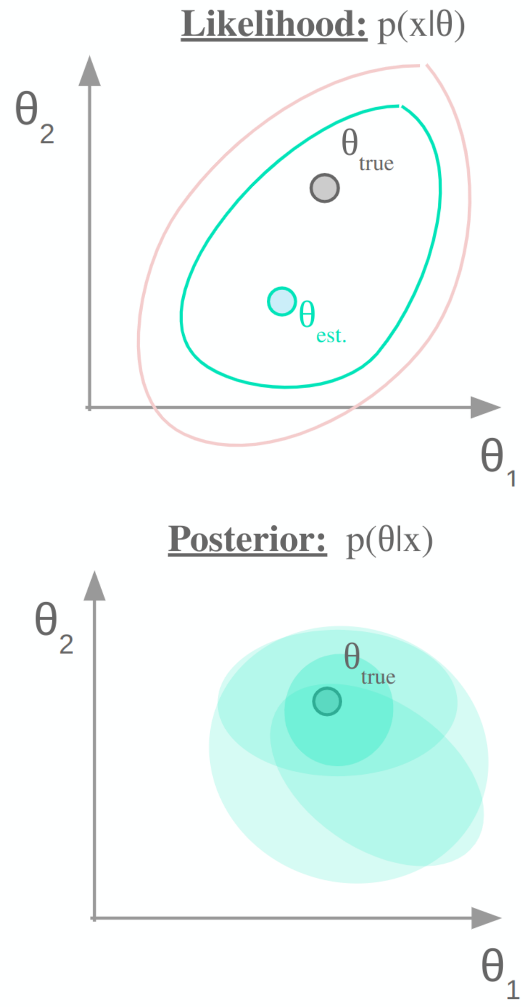

Estimators

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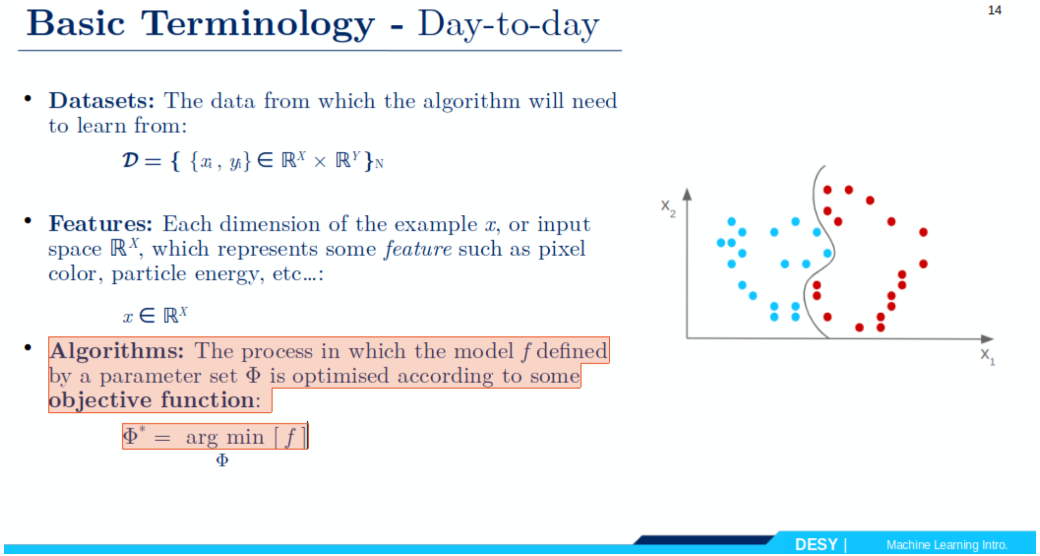
Recall on slide 14 of this lecture that from a mathematical perspective a ML model is the set of optimal parameter that match **data** *and* **predictions***!*



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- Is there a recipe for extracting from the data the optimal parameters or **best estimator?**

→ **Maximum Likelihood Method:**
General approach to estimating the point estimator

$$\hat{\theta} = \arg\max_{\theta} \; p(\{x\}_m|\theta)$$
$$= \arg\max_{\theta} \prod_{i}^{m} p(\; x \;|\theta)$$

Log-likelihood is preferred for numerical stability:

$$-\ln(\mathcal{L}(\theta|\{x\}_m)) = -\sum_{i}^{m} \ln p(x_i|\theta)$$

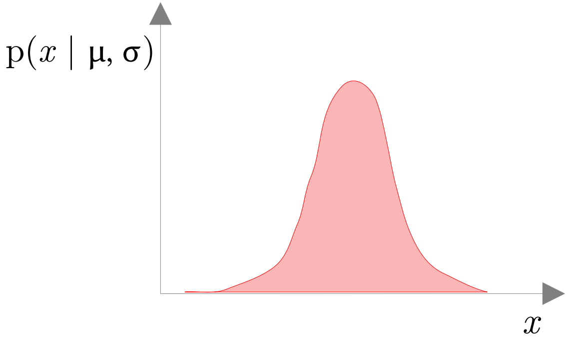
Guassian Estimator Example

Maximum Likelihood Method:

In a counting experiment, *model* data as Gaussian distributed:

$$p(x_i|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{1}{2}\frac{(x_i-\mu)^2}{\sigma^2}\right]$$

Model



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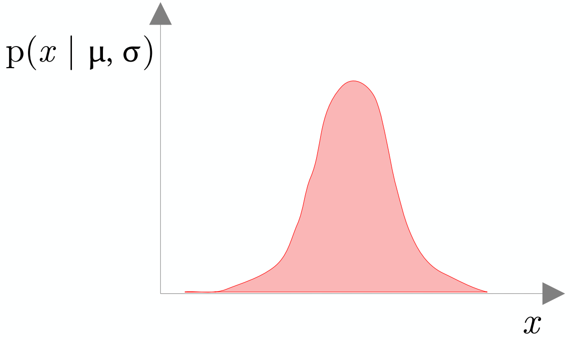

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We have some **data** $\mathbf{\{x\}_m}$ which forms an empirical distribution (more on this later), lets **maximise** the likelihood:

$$\frac{\partial}{\partial\theta}(-\ln\mathcal{L}(\theta|\{x\}_m)) \mapsto -\frac{1}{\sigma^2}\sum_i^m(x_i-\mu) = \sum_i^m x_i - m\mu = 0$$

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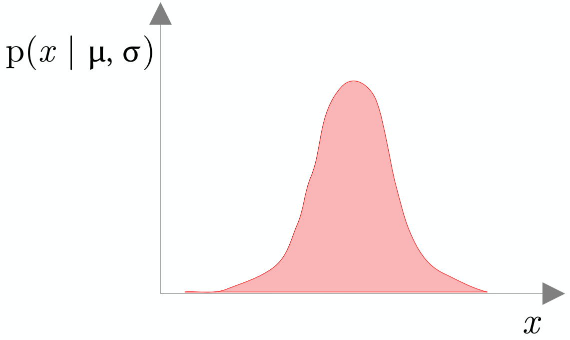

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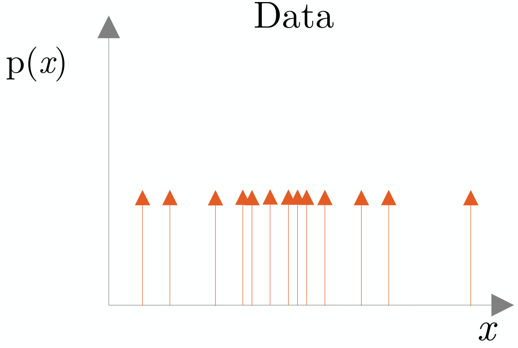

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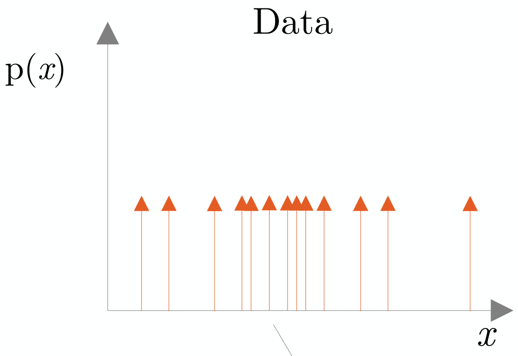

$$\hat{\mu} = \frac{1}{m}\sum_i^m x_i$$

With a bit of algebra we have derived the **sample mean**

Information Theory

- **Self-Information**:

$$I(x) = -\ln(P(x))$$

- **Uncertainty** in an entire distribution $P(x)$ – **Shannon Entropy:**

$$H(x) = \mathbb{E}_{x\sim P}\left[I(x)\right] = -\mathbb{E}_{x\sim P}\left[\ln(P(x))\right]$$

- **Relative Entropy** between two distributions $P(x)$ and $Q(x)$:

$$\mathcal{D}_{\mathrm{KL}}(P||Q) = \mathbb{E}_{x\sim P}\left[\ln\left(\frac{P(x)}{Q(x)}\right)\right]$$

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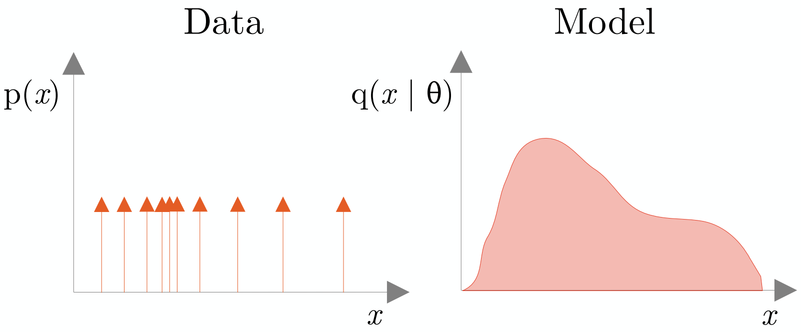
Key Points:

I) Data with low probability has high information content

II) Independent data samples are additive: $\mathrm{I}(x_1 \oplus x_2) = \mathrm{I}(x_1) + \mathrm{I}(x_2)$



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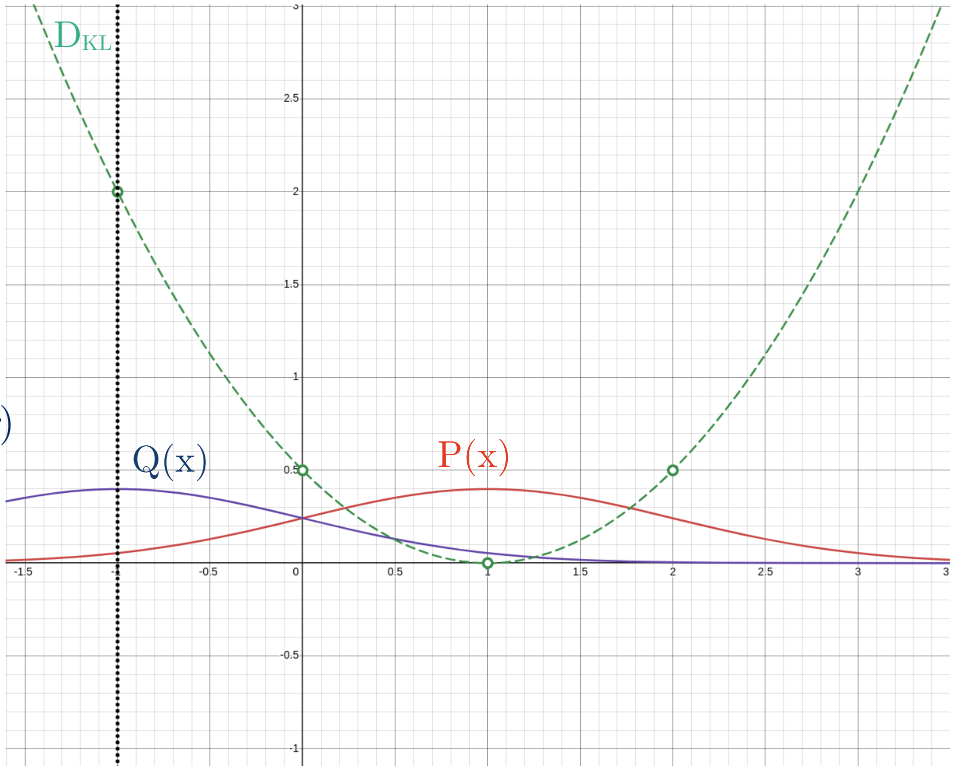

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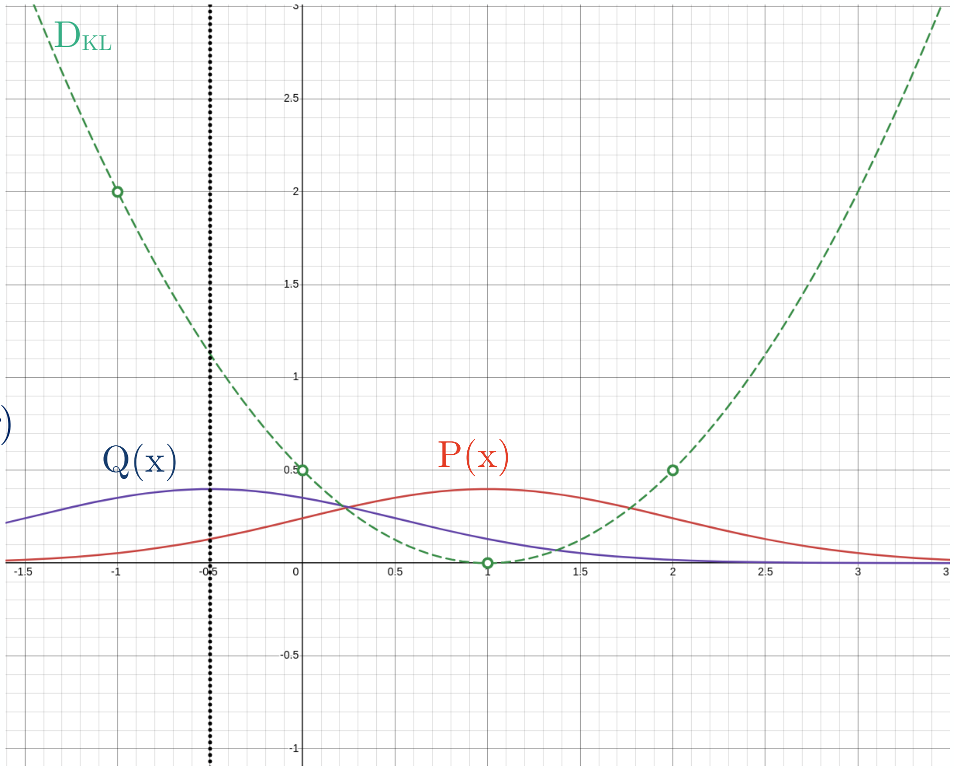

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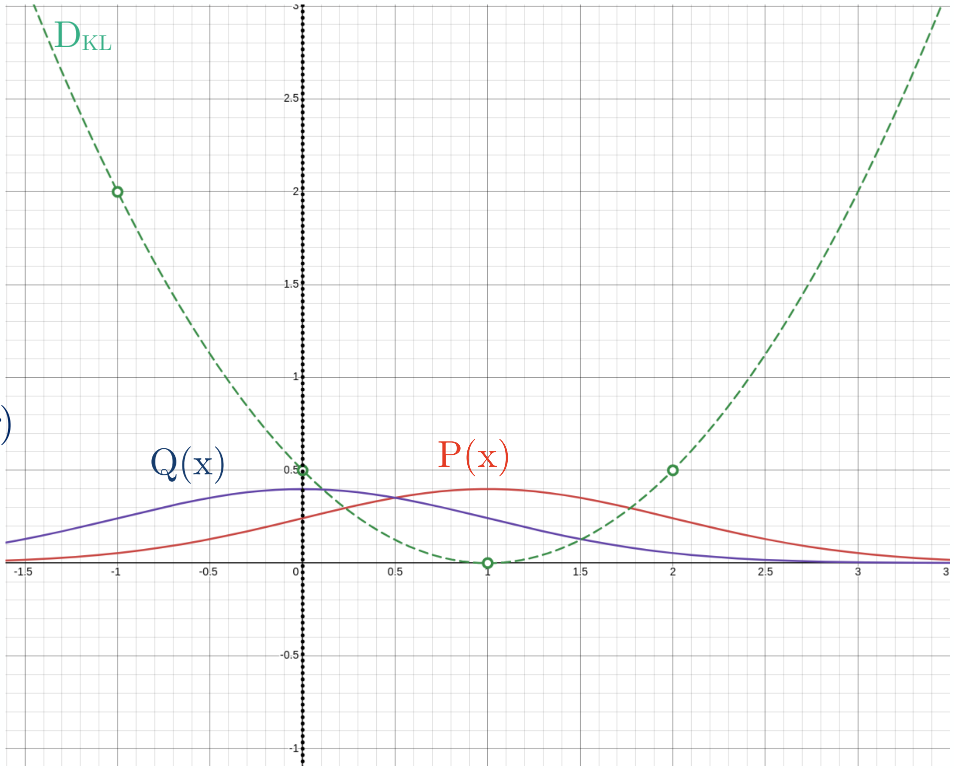

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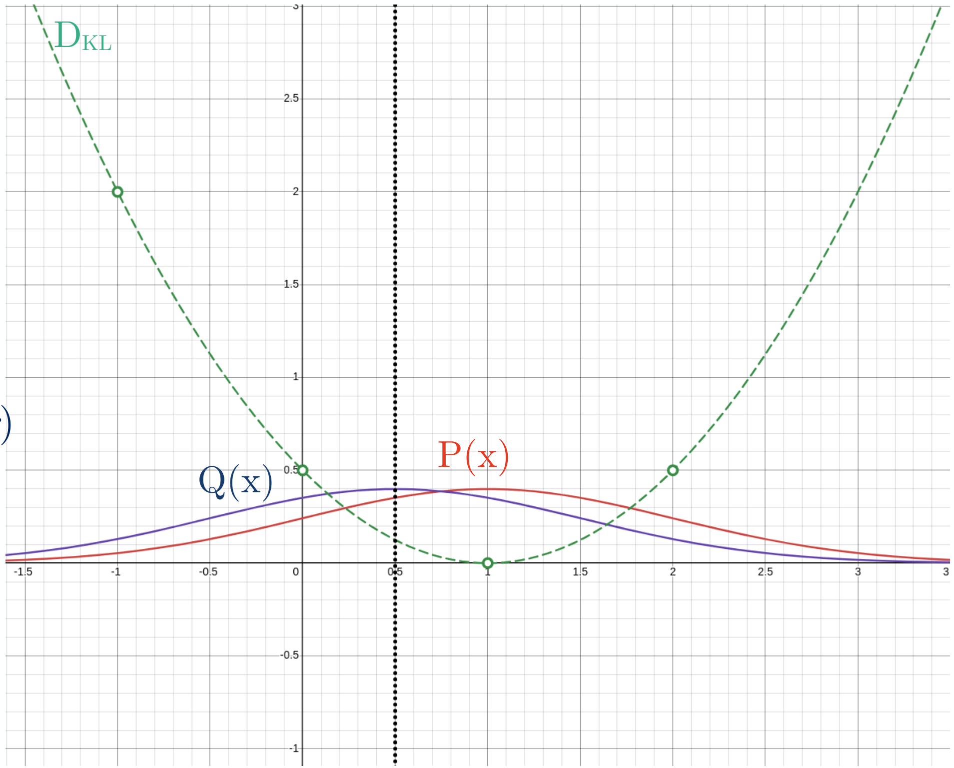

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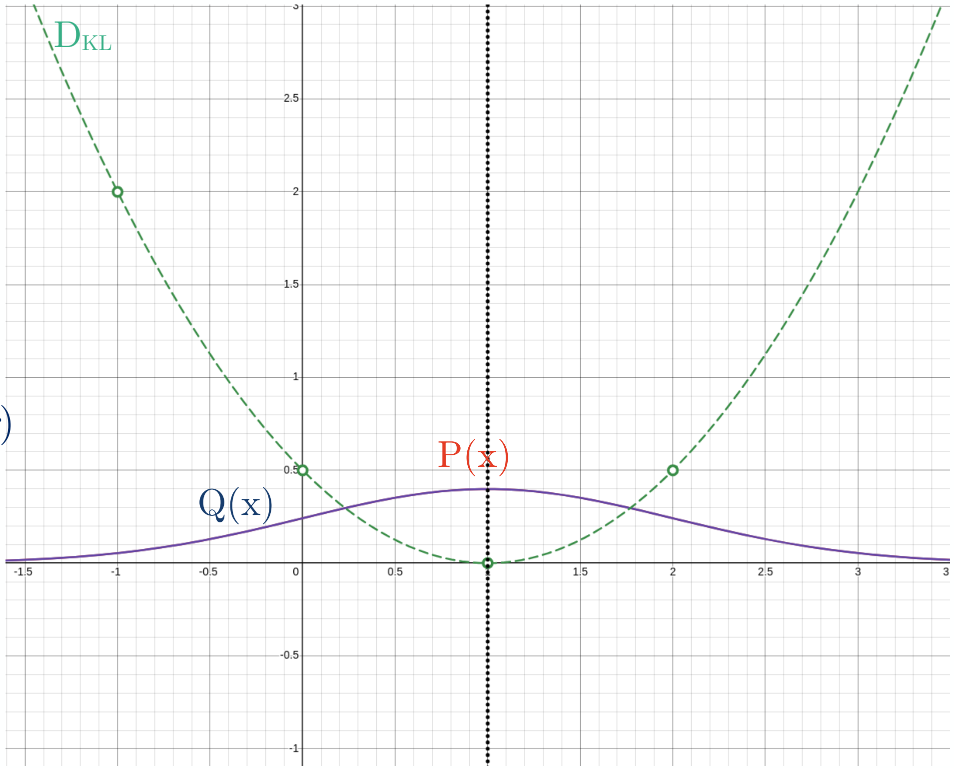

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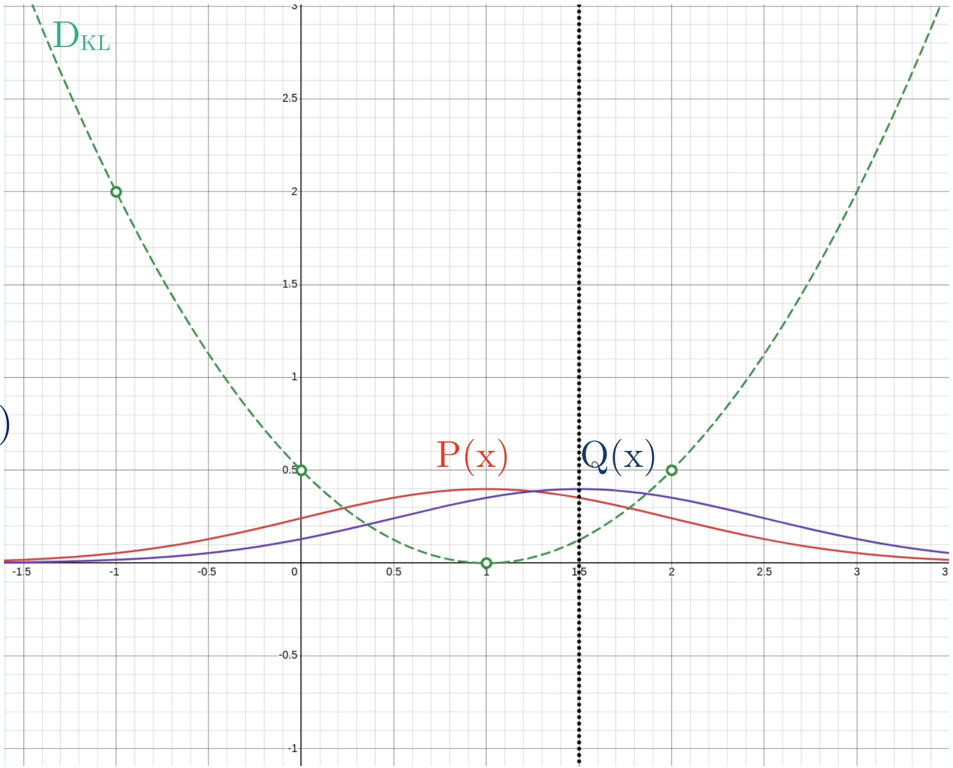

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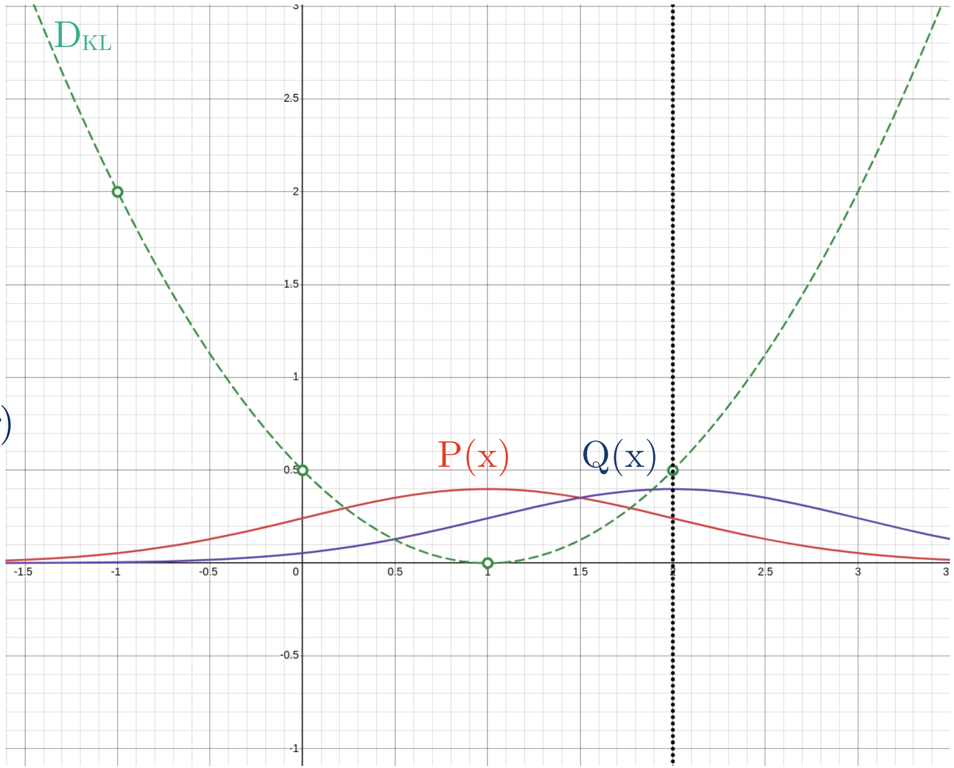

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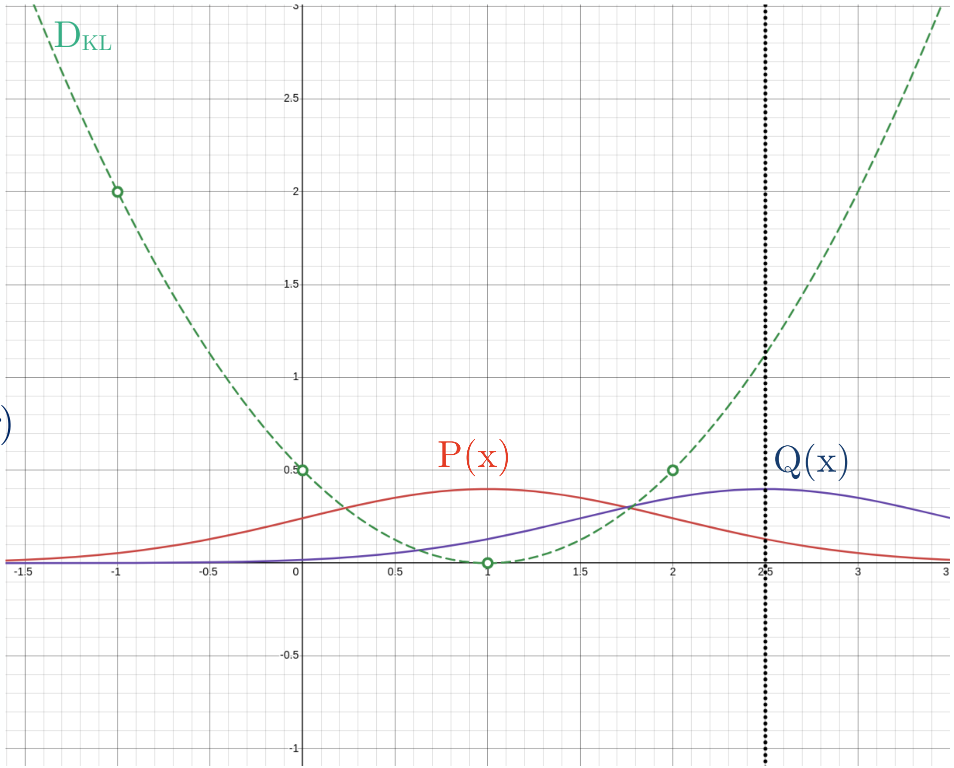

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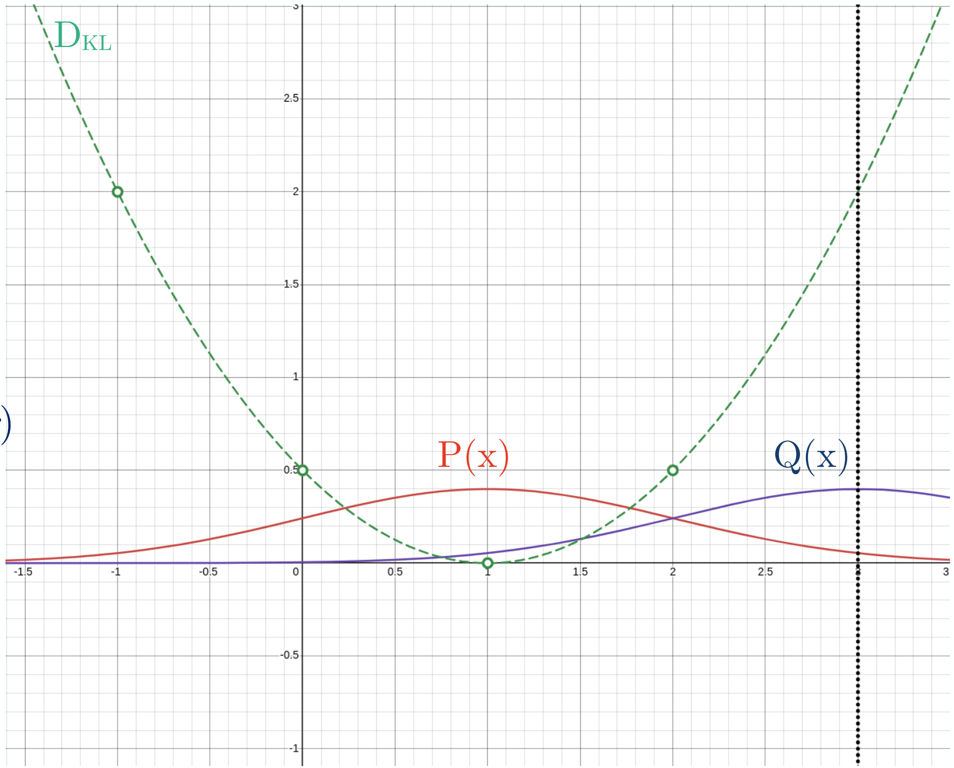

Maximum Likelihood Estimator

- **Intuitive understanding** of the maximum likelihood comes from the idea of *distance* between two distribution

$$\hat{\theta} = \arg\max_{\theta} \; \mathbb{E}_{x \sim p_{\text{data}}} \left[\log(p_{\text{model}}(x|\theta))\right]$$

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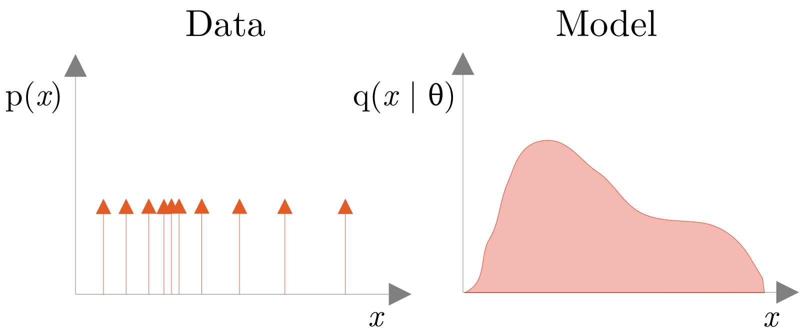

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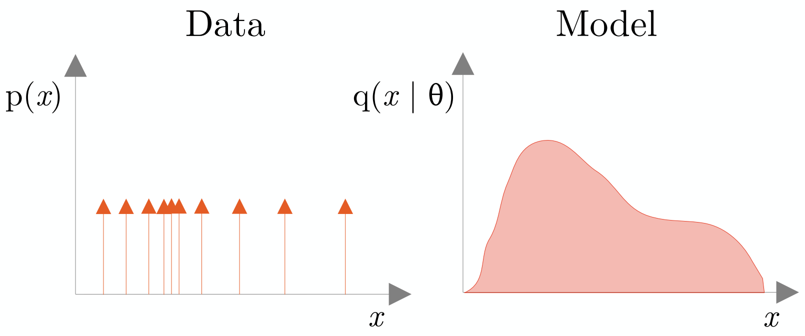

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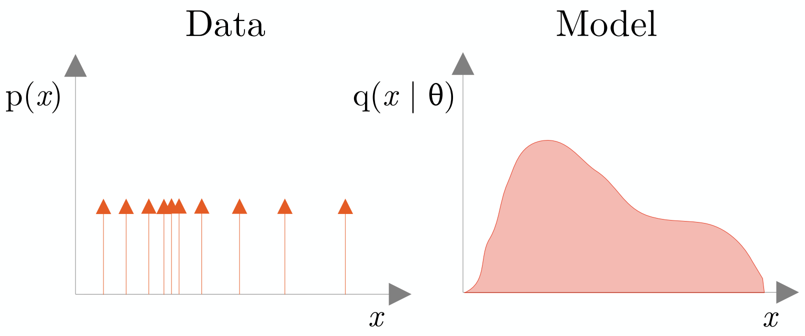

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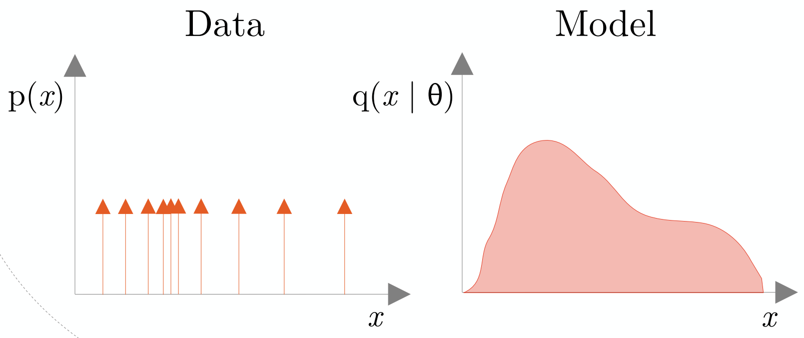

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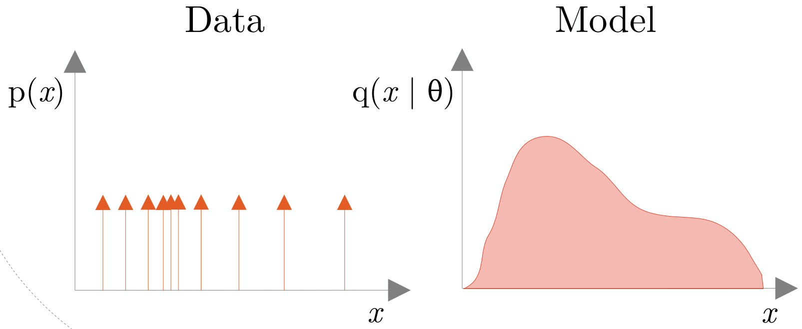

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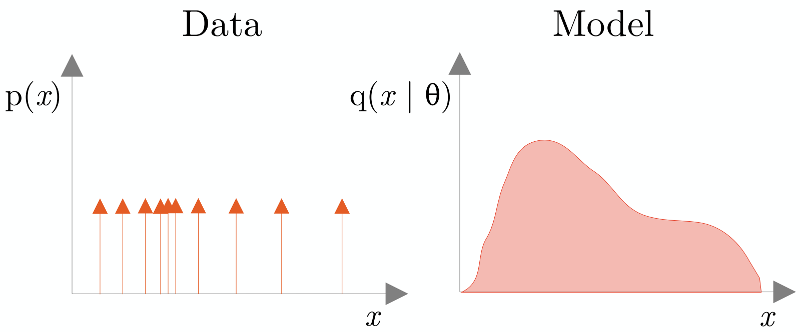

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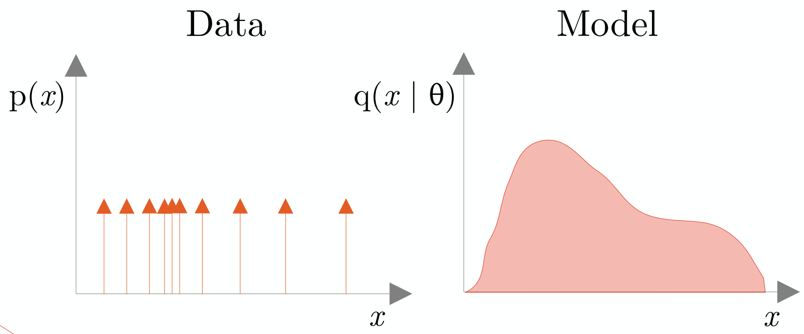

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Learning Process & Estimators

Learning Law

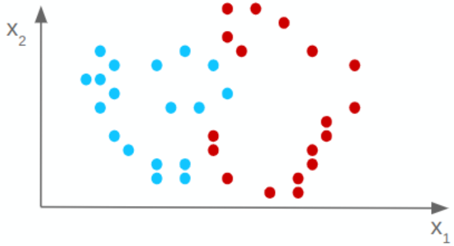
- **Four key parts** to the 'Machine Learning' process:

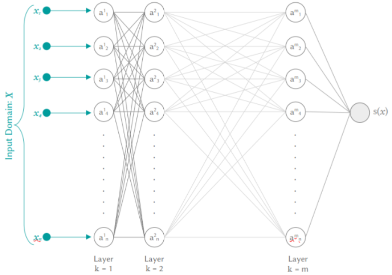
Dataset:
Supervised: $\mathcal{D} = \{ \{x_i , y_i\} \in \mathbb{R}^X \times \mathbb{R}^Y \}_N$
Unsupervised: $\mathcal{D} = \{ \{x_i\} \in \mathbb{R}^X \}_N$

Model f:
E.g. Neural network with parameters Φ

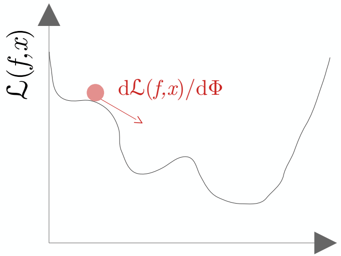
Loss/Cost Function $\mathcal{L}(f,x)$:
Function for calculating agreement between prediction of model and implicit data distribution

Optimise parameters Φ:
Optimisation algorithm





$$\mathcal{D}_{KL}(P||Q) = \mathbb{E}_{x\sim P}\left[\ln\left(P(x)\right) - \ln\left(Q(x)\right)\right]$$



Supervised vs Unsupervised

Dataset:
Supervised:
$\mathcal{D} = \{ \{x_i, y_i\} \in \mathbb{R}^X \times \mathbb{R}^Y \}_N$
Unsupervised:
$\mathcal{D} = \{ \{x_i\} \in \mathbb{R}^X \}_N$

- **Supervised** learning:
  Examples $\mathbf{x} = \{x\}_\mathrm{m}$ paired with targets $\mathrm{y} = \{y\}_\mathrm{m}$ that instruct the algorithm on what to learn

$$p(y|x)$$

- **Unsupervised** learning:
  Examples $\mathbf{x} = \{x\}_\mathrm{m}$ with no targets

$$p(x)$$

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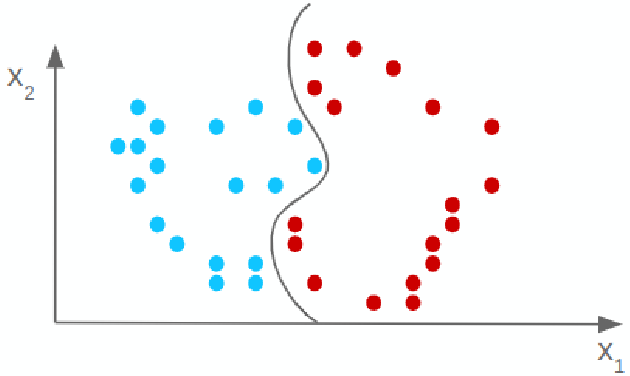
  $p(y|x)$ Conditional Density Estimation



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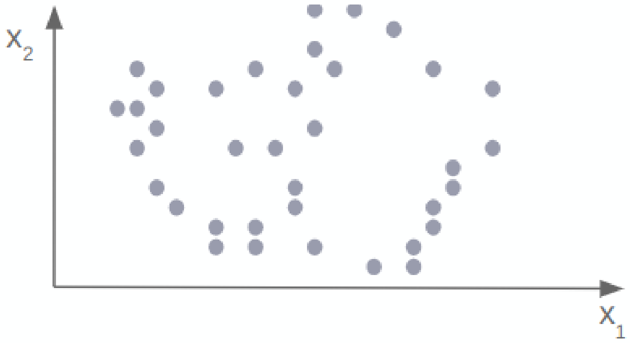
  $p(x)$ Density Estimation



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  $p(x)$ Density Estimation

Decomposing the problem into m-1 conditional density estimation problems ~ supervised learning problems

$$p(\{x\}_m) = \prod_i^m p(x_i|\{x\}_{m-i})$$

Supervised vs Unsupervised

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$p(y|x)$ Conditional Density Estimation

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  Examples $\mathbf{x} = \{x\}_m$ with no targets

$p(x)$ Density Estimation

$$p(\{y\}_m|\{x\}_m) = \frac{p(\{x\}_m, \{y\}_m)}{\sum_{\tilde{y}} p(\{x\}_m, \{\tilde{y}\}_m)}$$

Learning the joint distribution p(x,y) via unsupervised learning techniques, then infer.

Supervised vs Unsupervised

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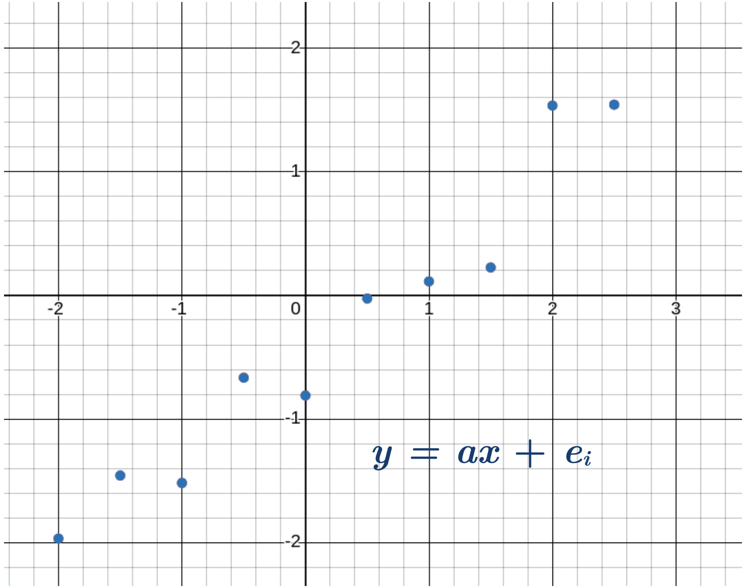


Linear Regression Example

Model

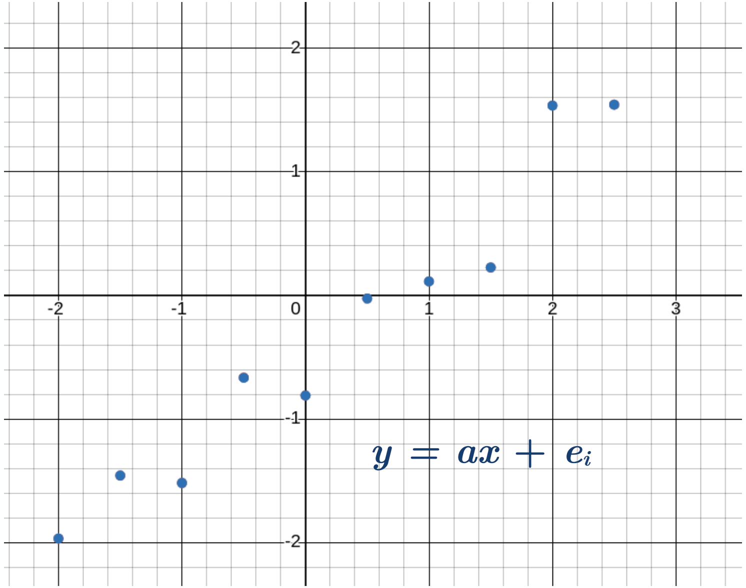
Model f:
E.g. Neural network with parameters Φ

- **Parametric linear model:**

$$\hat{y} = \boldsymbol{w}^T \mathbf{x}$$

- **Configurable parameters of model $\Phi = w$**

$$y = \begin{pmatrix} w_1, & \ldots, & w_n \end{pmatrix} \begin{pmatrix} x_1, \\ \cdot \\ \cdot \\ x_n \end{pmatrix}$$



Linear Regression Example

Performance Measure: Loss Function

Loss/Cost Function $\mathcal{L}(f,x)$:
Function for calculating agreement between prediction of model and implicit data distribution

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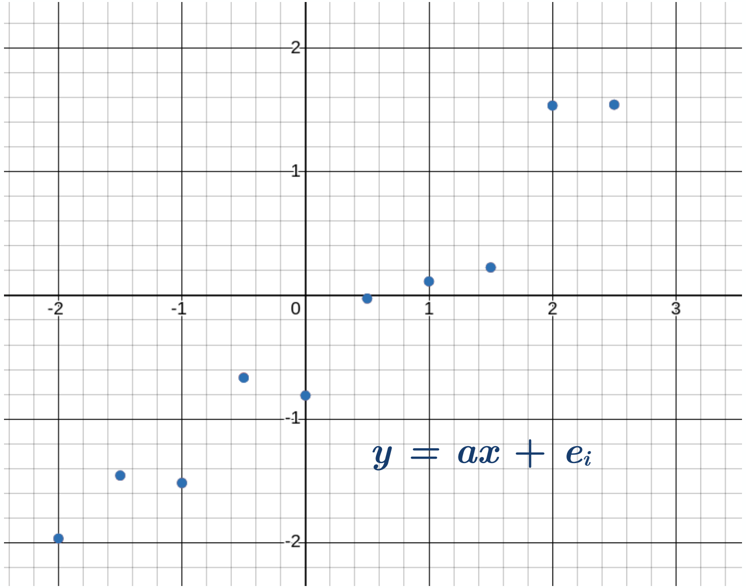
- **Loss:** Mean squared error

$$\mathcal{L} = \frac{1}{m} \sum_i (\hat{y} - y)^2$$



Linear Regression Example

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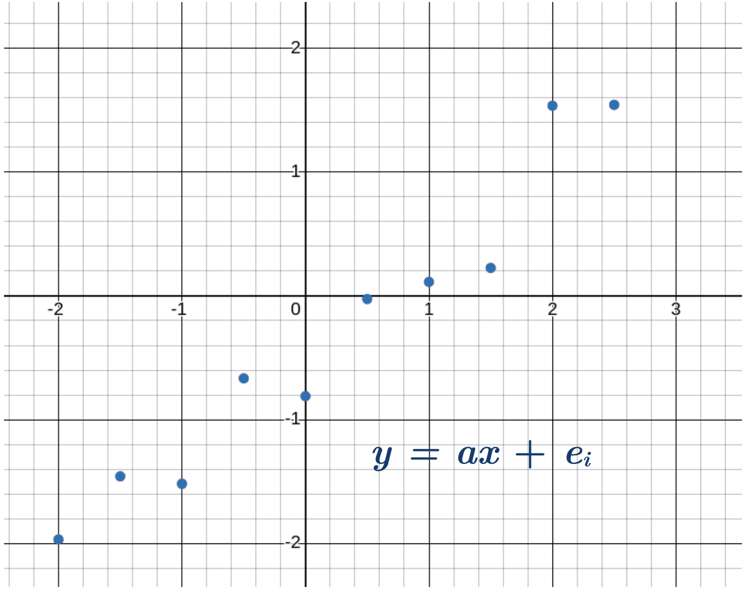
Why the mean squared error?



Linear Regression Example

Maximum Likelihood Approach

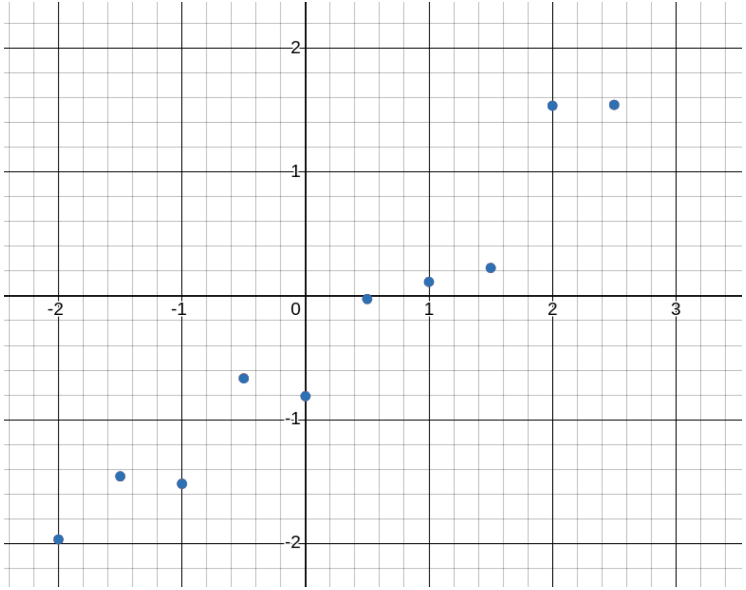
Optimise parameters Φ:
Optimisation algorithm

- I said there was a general likelihood approach to *estimating/learning* parameters:

$$\hat{\theta} = \arg\max_{\theta} \sum_{i}^{m} \ln p(x_i|\theta)$$

- **General MLE** estimate also applies to conditional probability:

$$\hat{\theta} = \arg\max_{\theta} \sum_{i}^{m} \ln \left(p(y_i|x_i, \theta)\right)$$



Linear Regression Example

Optimise parameters Φ:
Optimisation algorithm

Maximum Likelihood Approach

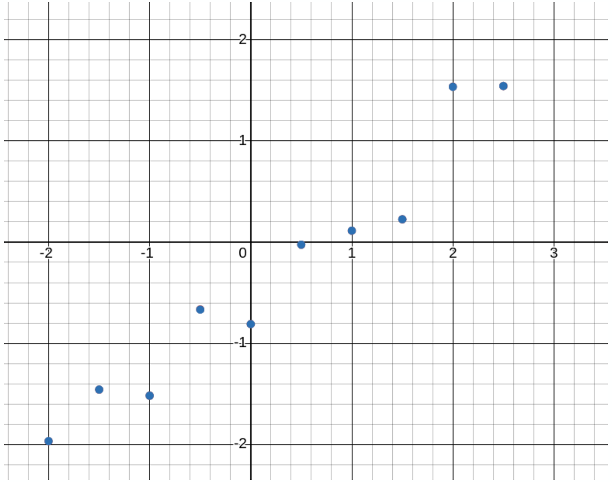
- **Probabilistic view of regression:**

  Data generated with an error term that is gaussian distributed, meaning repeated experiments have some noise:

$$y_i = \alpha x_i + e_i \quad \Rightarrow \quad y_i \sim \mathcal{N}(\alpha x_i, \sigma)$$

$$e_i \sim \mathcal{N}(0, \sigma)$$

Linear Regression Example



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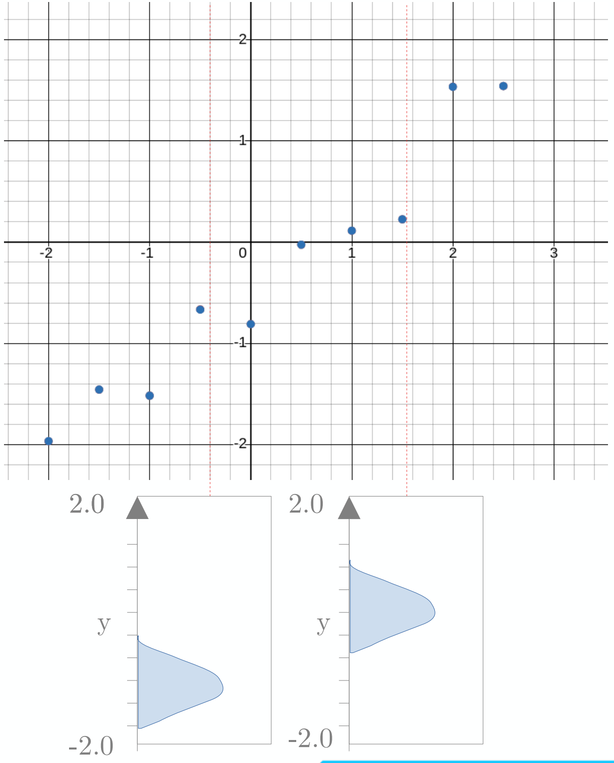

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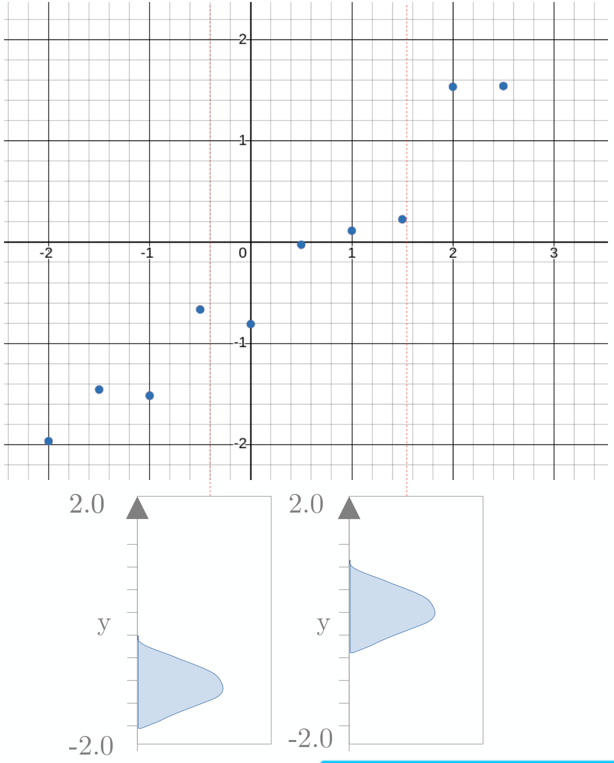
$$p(y_i|x_i, \alpha) = \mathcal{N}(y_i|\hat{y}_i, \sigma) = \mathcal{N}(y_i|\alpha x_i, \sigma)$$

Linear Regression Example



Maximum Likelihood Approach

Optimise parameters Φ:
Optimisation algorithm

- **Generalise MLE** estimate the conditional probability:

$$\hat{\theta} = \arg\max_{\theta} \sum_{i}^{m} \ln\left(p(y_i|x_i,\theta)\right)$$

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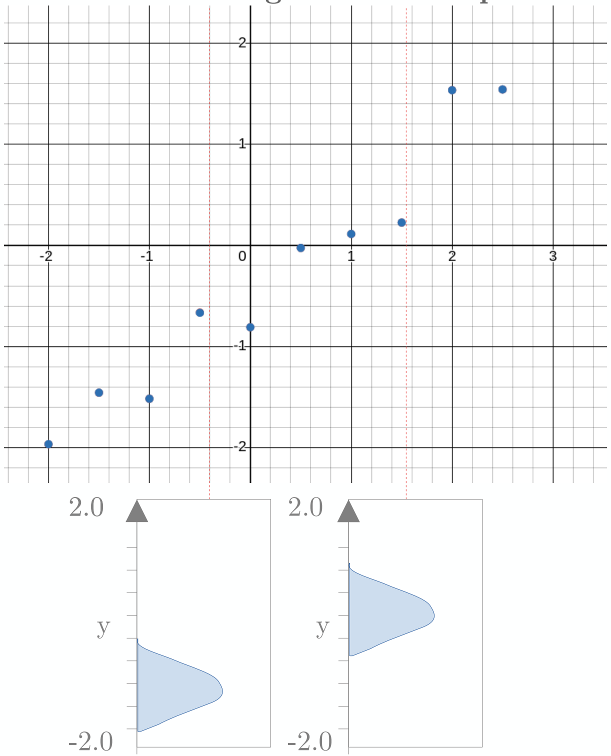
- **Probabilistic view of regression:**

$$\hat{\alpha} = \arg\max_{\theta} \sum_{i}^{m} \ln\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(\alpha x_i-\mu)^2}{2\sigma^2}}\right)$$

Linear Regression Example



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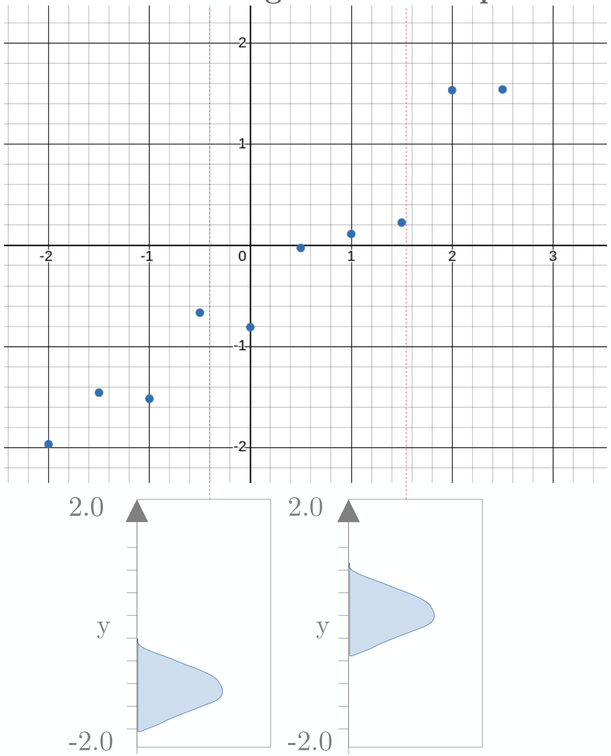
Linear Regression Example



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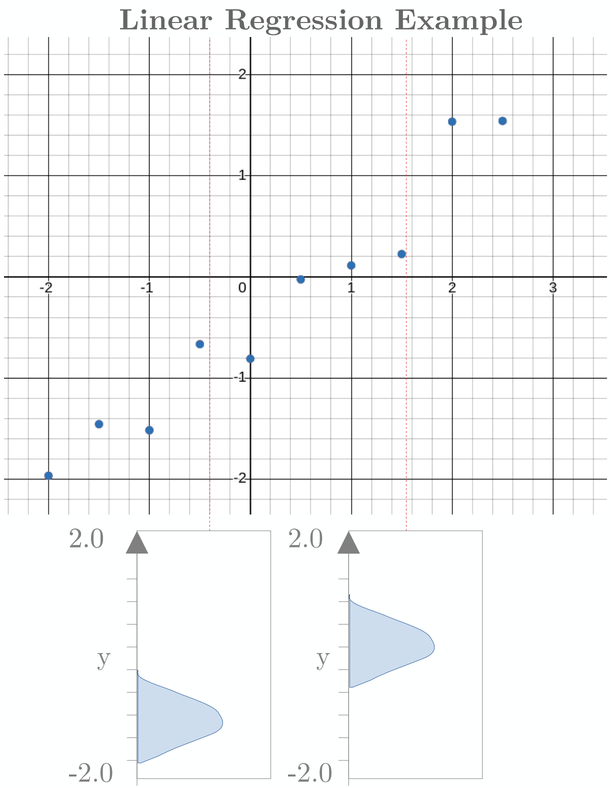


Gradient Descent

Optimise parameters Φ:

Optimisation algorithm

- **First Order Gradient Descent:**

$$\nabla_{\boldsymbol{w}} \mathrm{MSE}_{\mathrm{train}} = 0$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \frac{1}{m} ||\hat{\boldsymbol{y}}^{(\mathrm{train})} - \boldsymbol{y}^{(\mathrm{train})}||_2^2 = 0$$

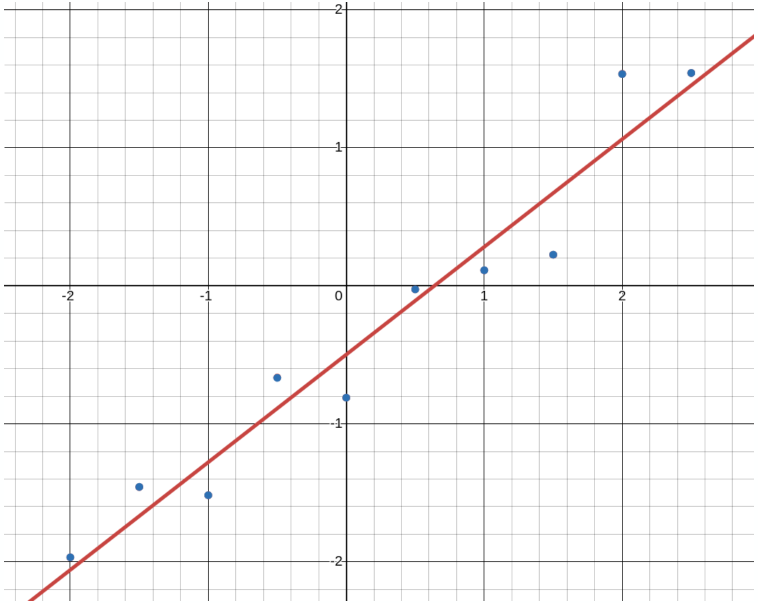
$$\Rightarrow \frac{1}{m} \nabla_{\boldsymbol{w}} ||\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}||_2^2 = 0$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\right)^\top \left(\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\right) = 0$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{w}^\top \boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{X}^{(\mathrm{train})} \boldsymbol{w} - 2\boldsymbol{w}^\top \boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})} + \boldsymbol{y}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})}\right) = 0$$

$$\Rightarrow 2\boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{X}^{(\mathrm{train})} \boldsymbol{w} - 2\boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})} = 0$$

$$\Rightarrow \boldsymbol{w} = \left(\boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{X}^{(\mathrm{train})}\right)^{-1} \boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})}$$



Linear Regression Example

Capacity & Bias-Variance Trade-Off

- **Capacity** of a model ~ the number of degrees of freedom that can be tuned

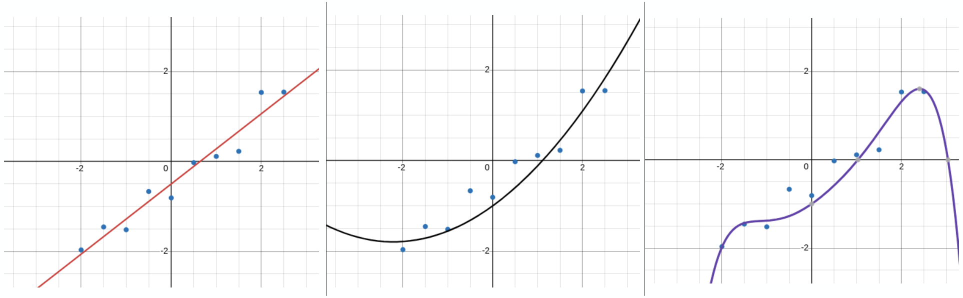
  1st Order Polynomial: $\hat{y} = wx + b$

  2nd Order Polynomial: $\hat{y} = w_1 x + w_2 x^2 + b$

  .

  .

  9th Order Polynomial: $\hat{y} = \sum_{i}^{9} w_i x^i + b$



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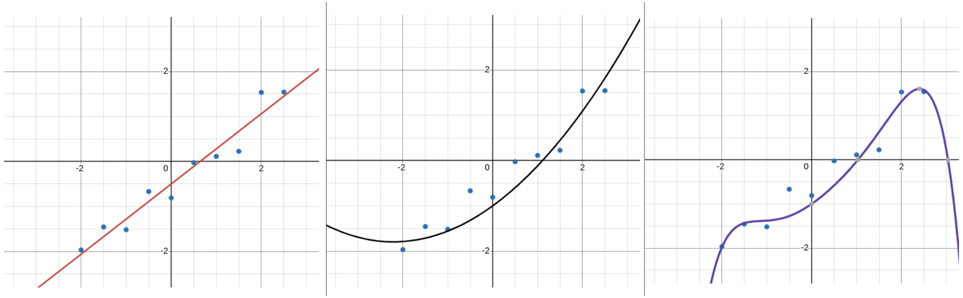
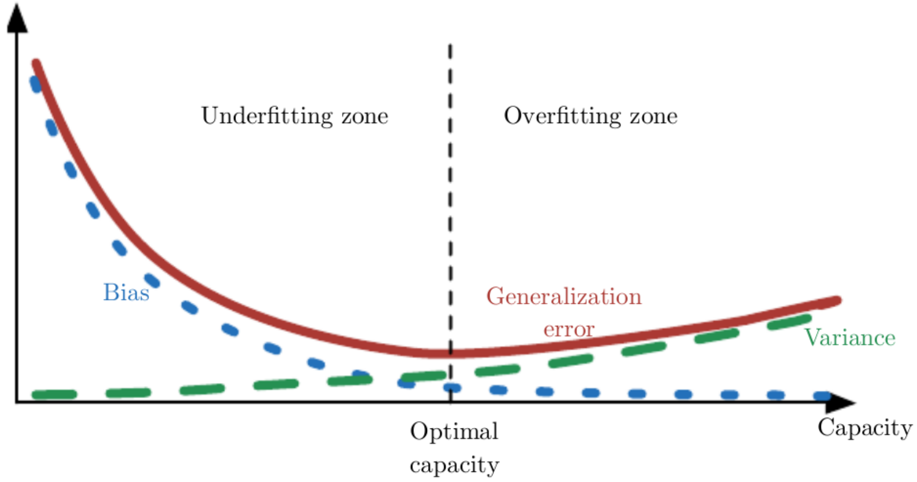
- **Under/Over-fitting** avoided by matching capacity of model to complexity of the problem





Estimators

- **Point Estimator, or statistic**, is any function of the data that infers from the data some parameter of interest θ:

$$\hat{\theta} = g(\{x\}_m)$$

- **Bias** of an estimator is given by:

$$\text{bias}(\hat{\theta}) = \mathbb{E}(\hat{\theta}) - \theta$$

- **Variance** of an estimator:

$$\text{Var}(\hat{\theta})$$

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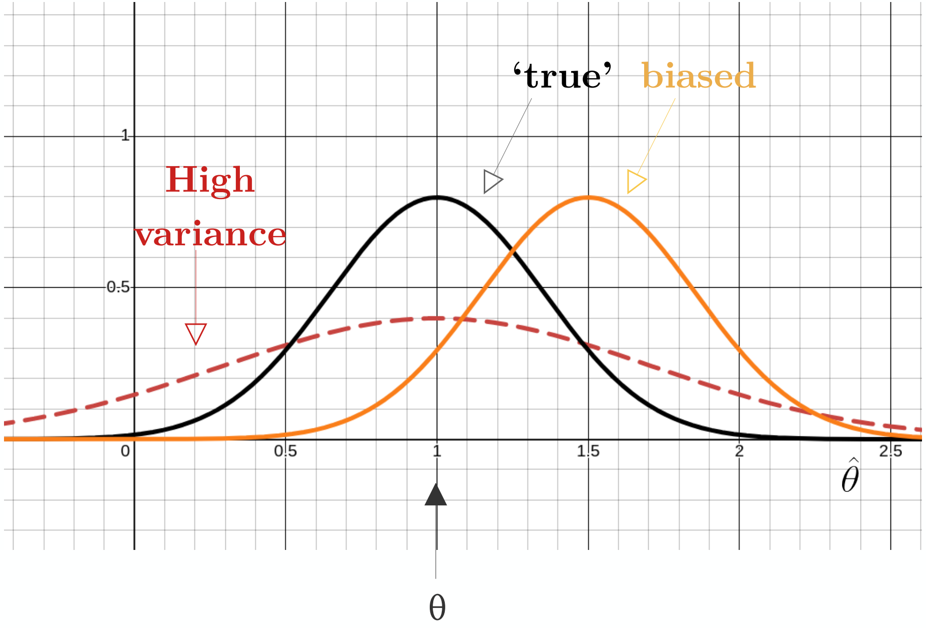
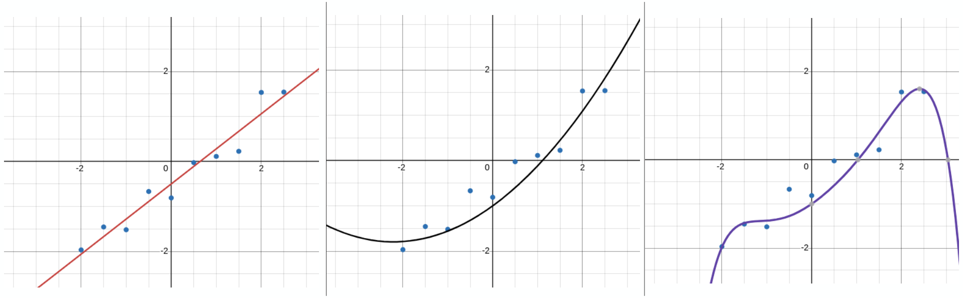
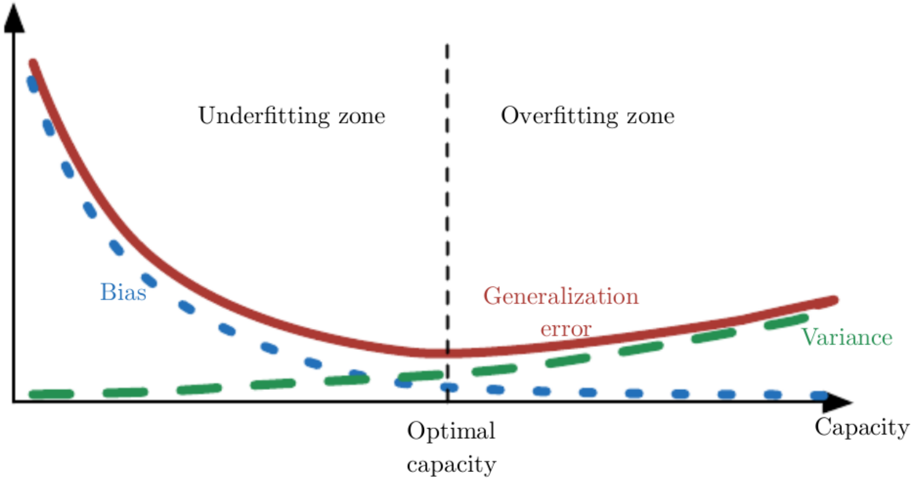


Capacity & Bias-Variance Trade-Off

- **Bias-Variance** trade-off:

$$
\begin{aligned}
\mathrm{MSE}(\hat{\theta},\theta) &= \mathbb{E}\left[(\hat{\theta}-\theta)^2\right] \\
&= \mathbb{E}\left[\hat{\theta}^2 - 2\hat{\theta}\theta + \theta^2\right] \\
&= \mathbb{E}\left[\hat{\theta}^2\right] - 2\mathbb{E}\left[\hat{\theta}\right]\theta + \theta^2 \\
&= \mathrm{Var}(\hat{\theta}) + \mathbb{E}\left[\hat{\theta}\right]^2 - 2\mathbb{E}\left[\hat{\theta}\right]\theta + \theta^2 \\
&= \mathrm{Var}(\hat{\theta}) + \mathrm{bias}(\hat{\theta})^2
\end{aligned}
$$

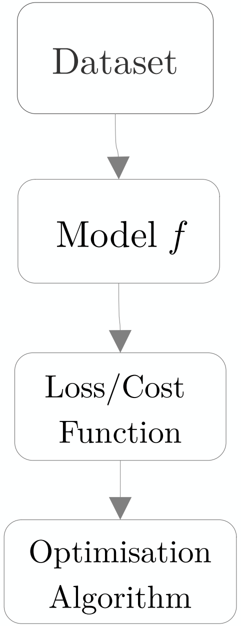




Learning Recipe

Recap

General recipe for *most* ML algorithms or learning processes:



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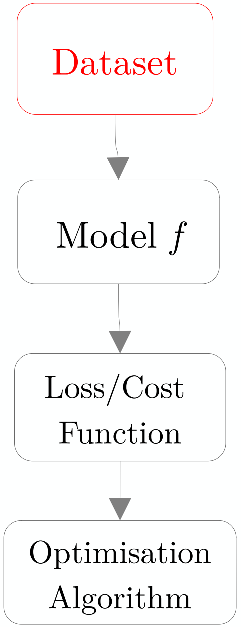

Experience

- **Supervised** learning:
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- **Unsupervised** learning:
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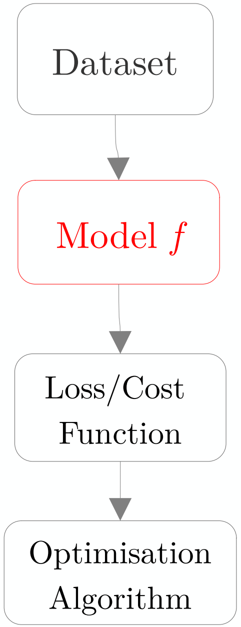

Task

- **Parametric linear model:**

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- **Configurable parameters of model $\Phi = w$**

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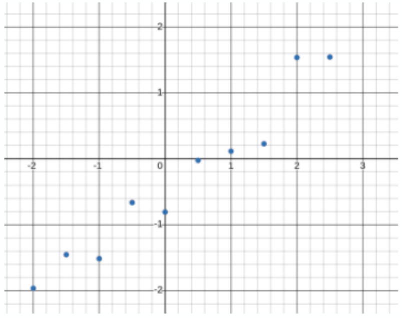

Linear Regression Example

Recap

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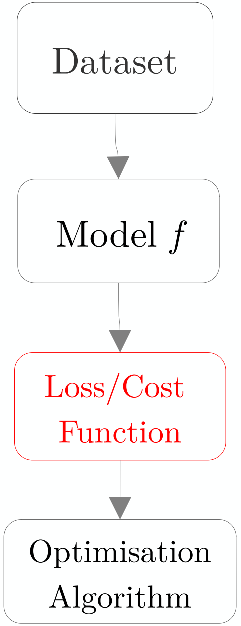

Performance

- **Generalise MLE** estimate the conditional probability:

$$\hat{\theta} = \arg\max_{\theta} \sum_{i}^{m} \ln\left(p(y_i | x_i, \theta)\right)$$

- **Probabilistic view of regression:**

$$\hat{m} = \arg\max_{\theta} \sum_{i}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(\alpha x_i - y_i)^2}{2\sigma^2}}$$

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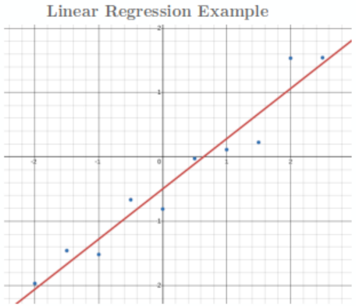

- **Maximising** the log-likelihood is equivalent to MSE minimisation

Recap

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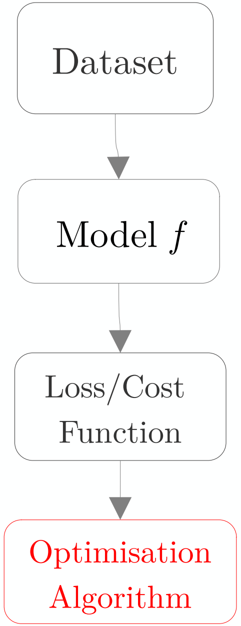


- **First Order Gradient Descent:**

$$\nabla_{\boldsymbol{w}} \mathrm{MSE}_{\mathrm{train}} = 0 \tag{5.6}$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\mathrm{train})} - \boldsymbol{y}^{(\mathrm{train})}\|_2^2 = 0 \tag{5.7}$$

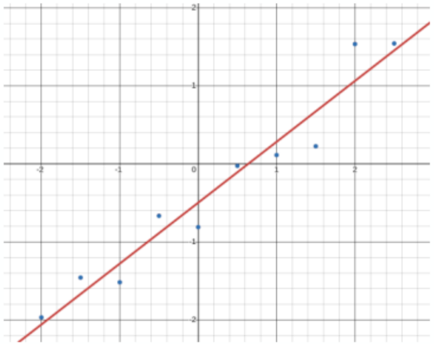
$$\Rightarrow \frac{1}{m} \nabla_{\boldsymbol{w}} \|\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\|_2^2 = 0 \tag{5.8}$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\right)^\top \left(\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\right) = 0 \tag{5.9}$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{w}^\top \boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{X}^{(\mathrm{train})} \boldsymbol{w} - 2\boldsymbol{w}^\top \boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})} + \boldsymbol{y}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})}\right) = 0 \tag{5.10}$$

$$\Rightarrow 2\boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{X}^{(\mathrm{train})} \boldsymbol{w} - 2\boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})} = 0 \tag{5.11}$$

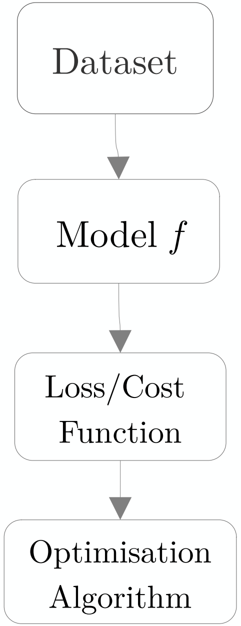
$$\Rightarrow \boldsymbol{w} = \left(\boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{X}^{(\mathrm{train})}\right)^{-1} \boldsymbol{X}^{(\mathrm{train})\top} \boldsymbol{y}^{(\mathrm{train})} \tag{5.12}$$



Linear Regression Example

Recap

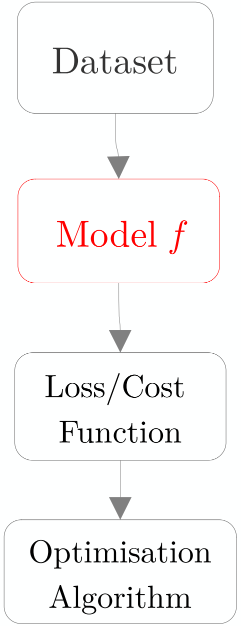
General recipe for *most* ML algorithms or learning processes:



Are we done?

Recap

General recipe for *most* ML algorithms or learning processes:



Are we done?

- How do we change the **family of functions** that a model learns? Scale capacity?

- **Capacity** of a model ~ the number of degrees of freedom that can be tuned

  1^{st} Order Polynomial: $\hat{y} = wx + b$

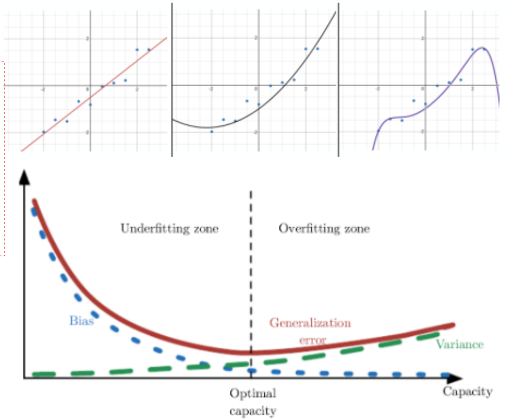
  2^{nd} Order Polynomial: $\hat{y} = w_1 x + w_2 x^2 + b$

  .

  .

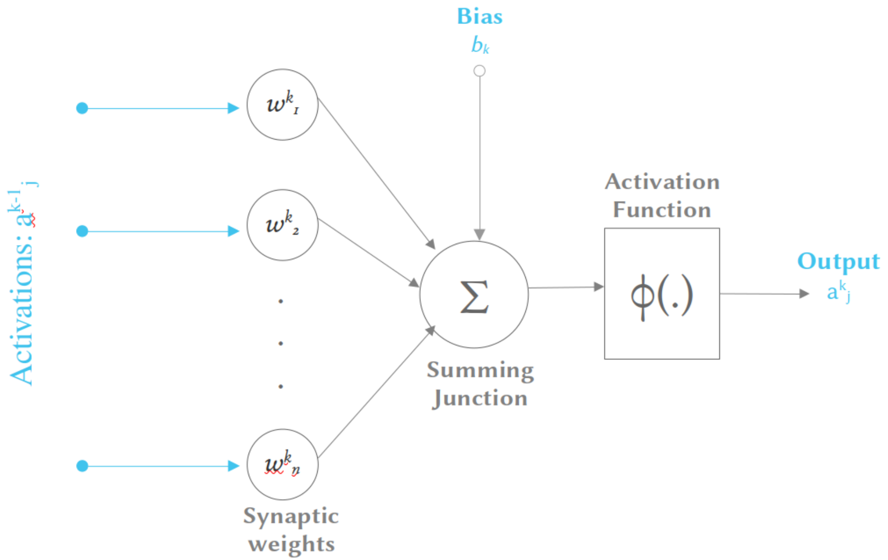
  9^{th} Order Polynomial: $\hat{y} = \sum_i^9 w_i x^i + b$

- **Under/Over-fitting** avoided by matching capacity of model to complexity of the problem



Neural Networks

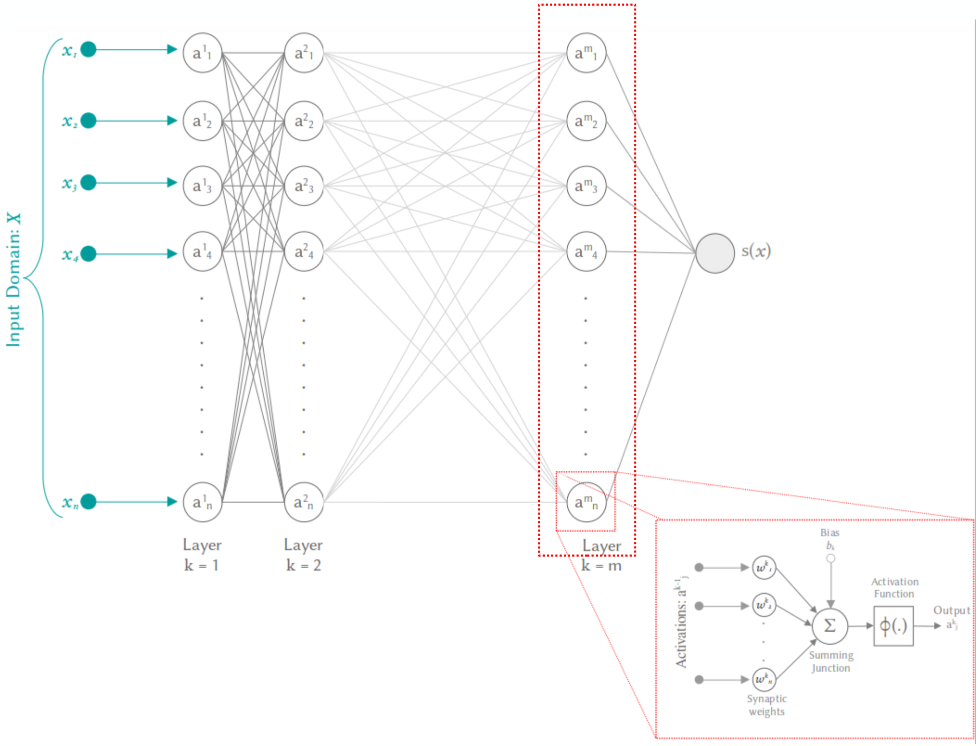
Neuron



- **Building block** of neural networks:

$$a_i^{(k+1)} = \phi\left(\sum_j^n w_{i,j}^{(k)} a_j^{(k)} + b^{(k)}\right)$$

Neuron → Layer



- **Building block** of neural networks:

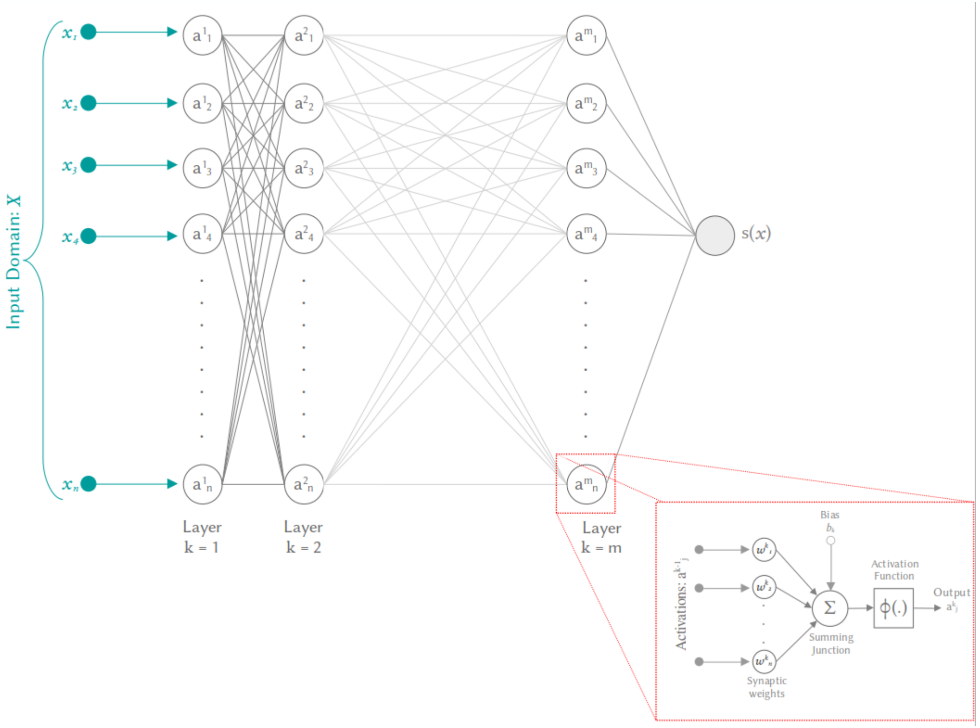
$$a_i^{(k+1)} = \phi\left(\sum_j^n w_{i,j}^{(k)} a_j^{(k)} + b^{(k)}\right)$$

Where, $a^{(k)}_i$ is the activation value, and the $\Phi=\{w^{(k)}_i, b^{(k)}\}$ are the configurable weights & biases

- **Neural Network** layer is the combination of many neurons densely connected (mostly…):

$$\begin{bmatrix} a_0^{(k+1)} \\ \dots \\ a_n^{(k+1)} \end{bmatrix} = \phi\left(\begin{bmatrix} w_0^{(0)} & \dots & w_n^{(0)} \\ \dots & \dots & \dots \\ w_0^{(k)} & & w_n^{(k)} \end{bmatrix} \begin{bmatrix} a_0^{(k)} \\ \dots \\ a_n^{(k)} \end{bmatrix} + \begin{bmatrix} b_0^{(k)} \\ \dots \\ b_n^{(k)} \end{bmatrix}\right)$$

Neural Network

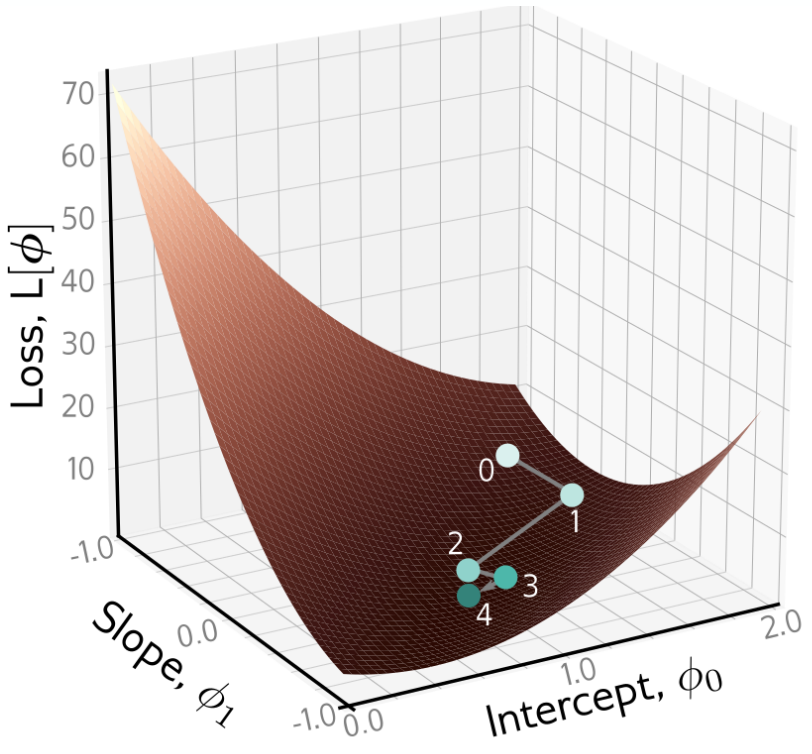


- A **total network** is therefore:

$$\mathbf{a}^{(1)} = \phi\left(\mathbf{W}^{(0)}\mathbf{x} + \beta^{(0)}\right)$$
$$\vdots$$
$$\mathbf{a}^{(k)} = \phi\left(\mathbf{W}^{(k-1)}\mathbf{a}^{(k-1)} + \beta^{(k-1)}\right)$$
$$\vdots$$
$$\mathbf{s}(\mathbf{x}) = \mathbf{W}^{(k)}\mathbf{a}^{(k)} + \beta^{(k)}$$

- ϕ is the activation function, which can take many forms
- Optimisation is done via typically gradient based descent algorithms

Stochastic Gradient Descent



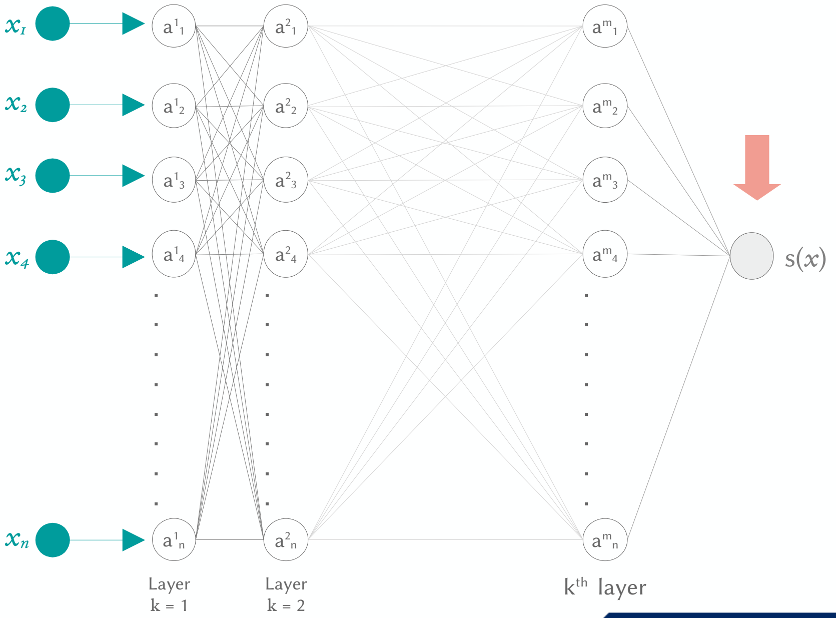
- **Stochastic Gradient Descent** is an adaptation of gradient descent:
  1) Calculate gradients:
  $$\frac{\partial \mathcal{L}}{\partial \Phi} = \begin{bmatrix} \frac{d\mathcal{L}}{\partial \phi_0} \\ \dots \\ \frac{d\mathcal{L}}{\partial \phi_h} \end{bmatrix}$$
  2) Update the parameters in direction that minimises loss:
  $$\phi_i^{(t+1)} \leftarrow \phi_i^{(t)} - \alpha . \sum_{j \in \mathcal{B}_t} \frac{\partial \mathcal{L}_j}{\partial \phi_{i,j}^{(t)}}$$
- **Batch based** training with iterative updates to the gradients based on an **epoch** 't', but the key goal is to learn:

$$\frac{\partial \mathcal{L}_j}{d\beta_j^{(k)}} \qquad \frac{\partial \mathcal{L}_j}{d\mathbf{W}_j^{(k)}}$$

Backwards Propagation – Optimisation Algorithm

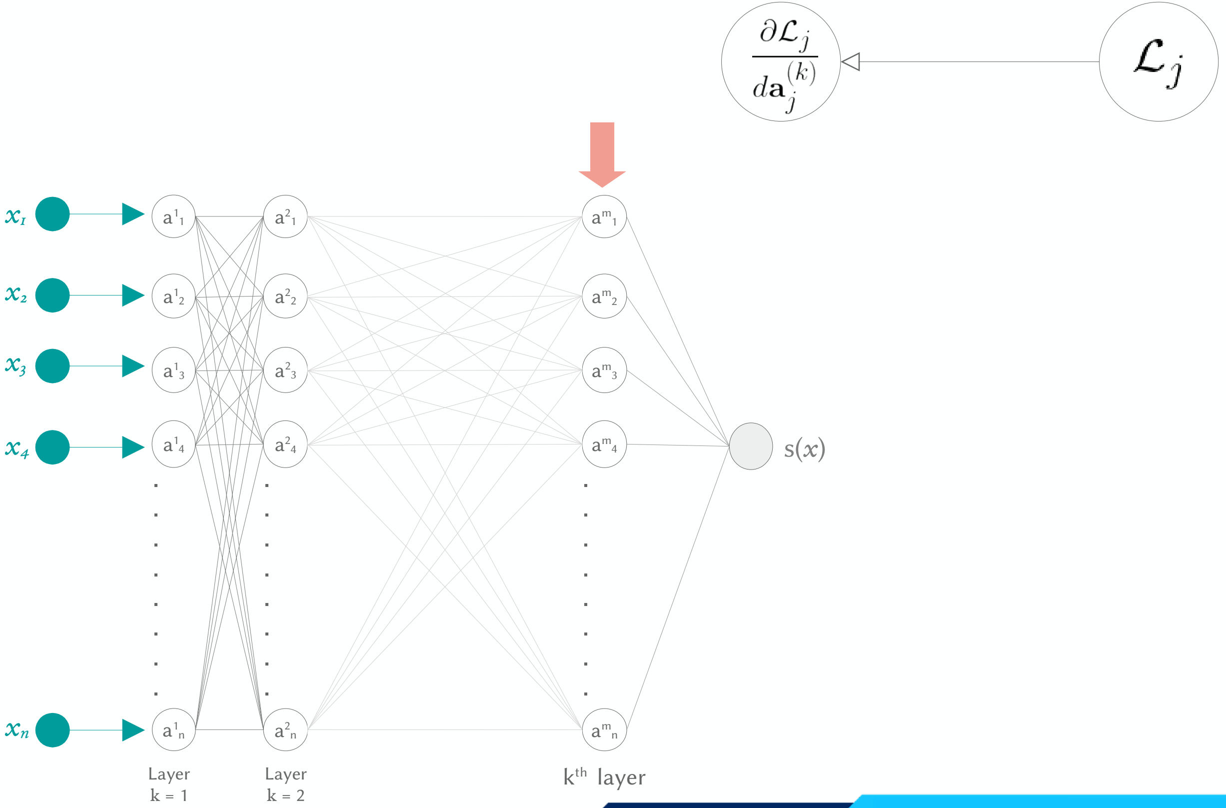
$$\mathbf{s}(\mathbf{x}) = \mathbf{W}^{(k)}\mathbf{a}^{(k)} + \beta^{(k)}$$

$\mathcal{L}_j$



Backwards Propagation – Optimisation Algorithm

$$\mathbf{a}^{(k)} = \phi\left(\mathbf{W}^{(k-1)}\mathbf{a}^{(k-1)} + \beta^{(k-1)}\right) \qquad \mathbf{s}(\mathbf{x}) = \mathbf{W}^{(k)}\mathbf{a}^{(k)} + \beta^{(k)}$$



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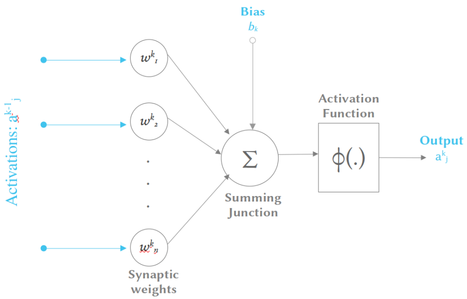
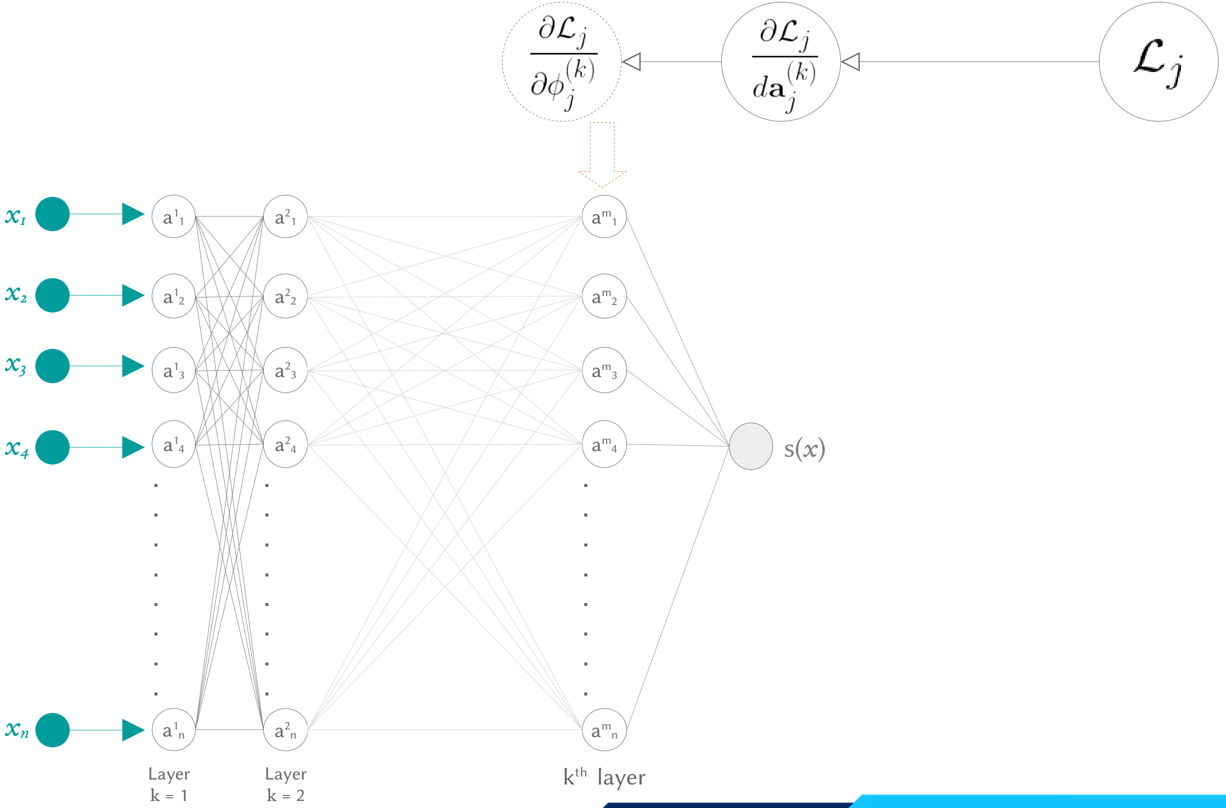
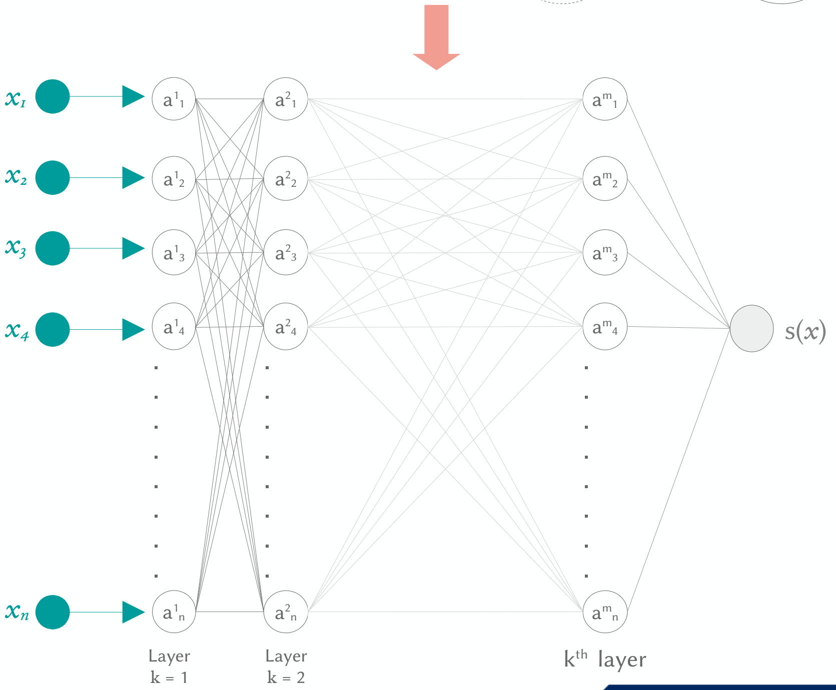




Backwards Propagation – Optimisation Algorithm

$$\mathbf{a}^{(k)} = \phi\left(\mathbf{W}^{(k-1)}\mathbf{a}^{(k-1)} + \beta^{(k-1)}\right) \qquad \mathbf{s}(\mathbf{x}) = \mathbf{W}^{(k)}\mathbf{a}^{(k)} + \beta^{(k)}$$

$$\cdots\cdots \leftarrow \frac{\partial \mathcal{L}_j}{\partial \phi_j^{(k)}} \leftarrow \frac{\partial \mathcal{L}_j}{d\mathbf{a}_j^{(k)}} \leftarrow \mathcal{L}_j$$



Backwards Propagation – Optimisation Algorithm

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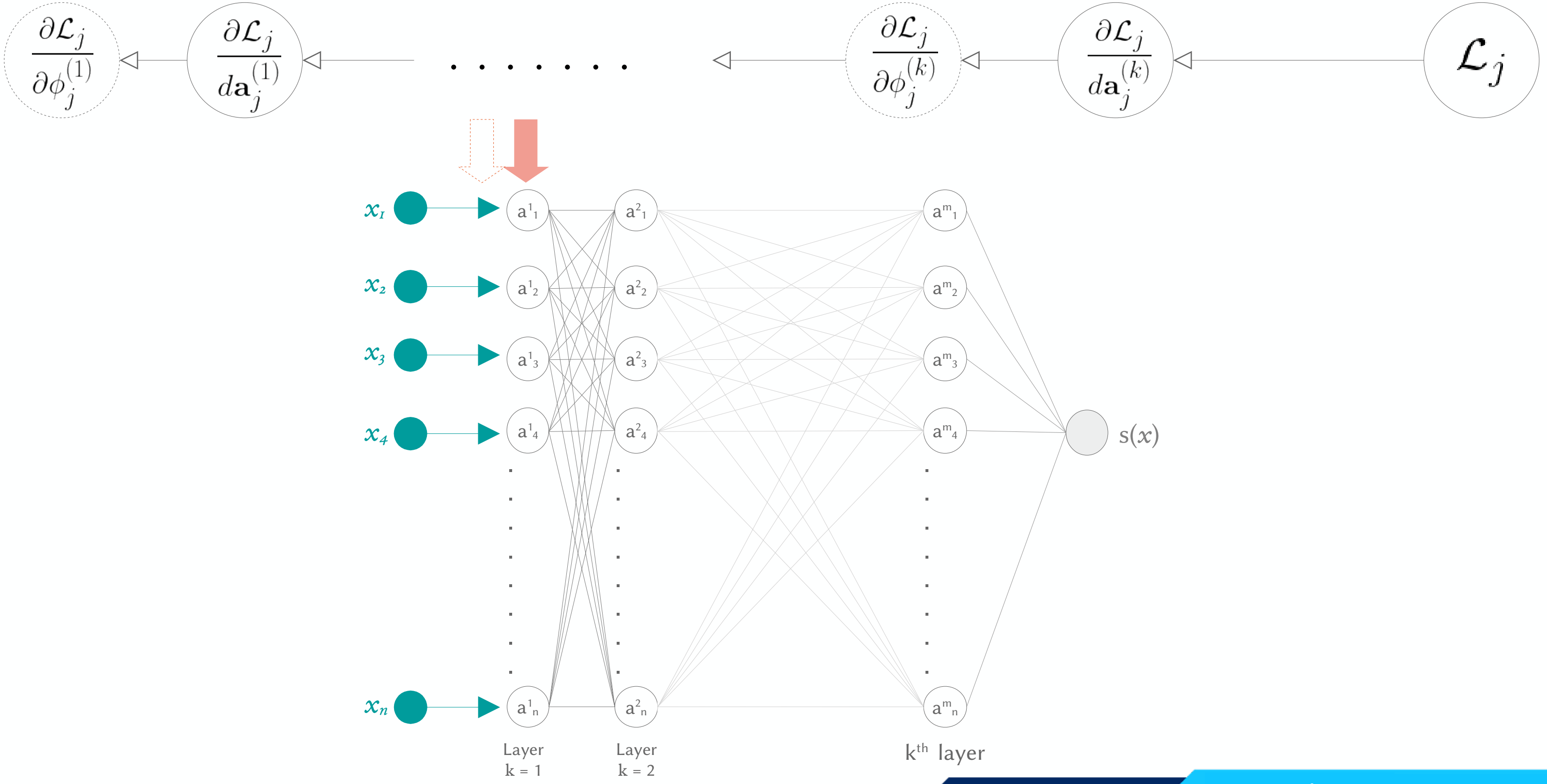
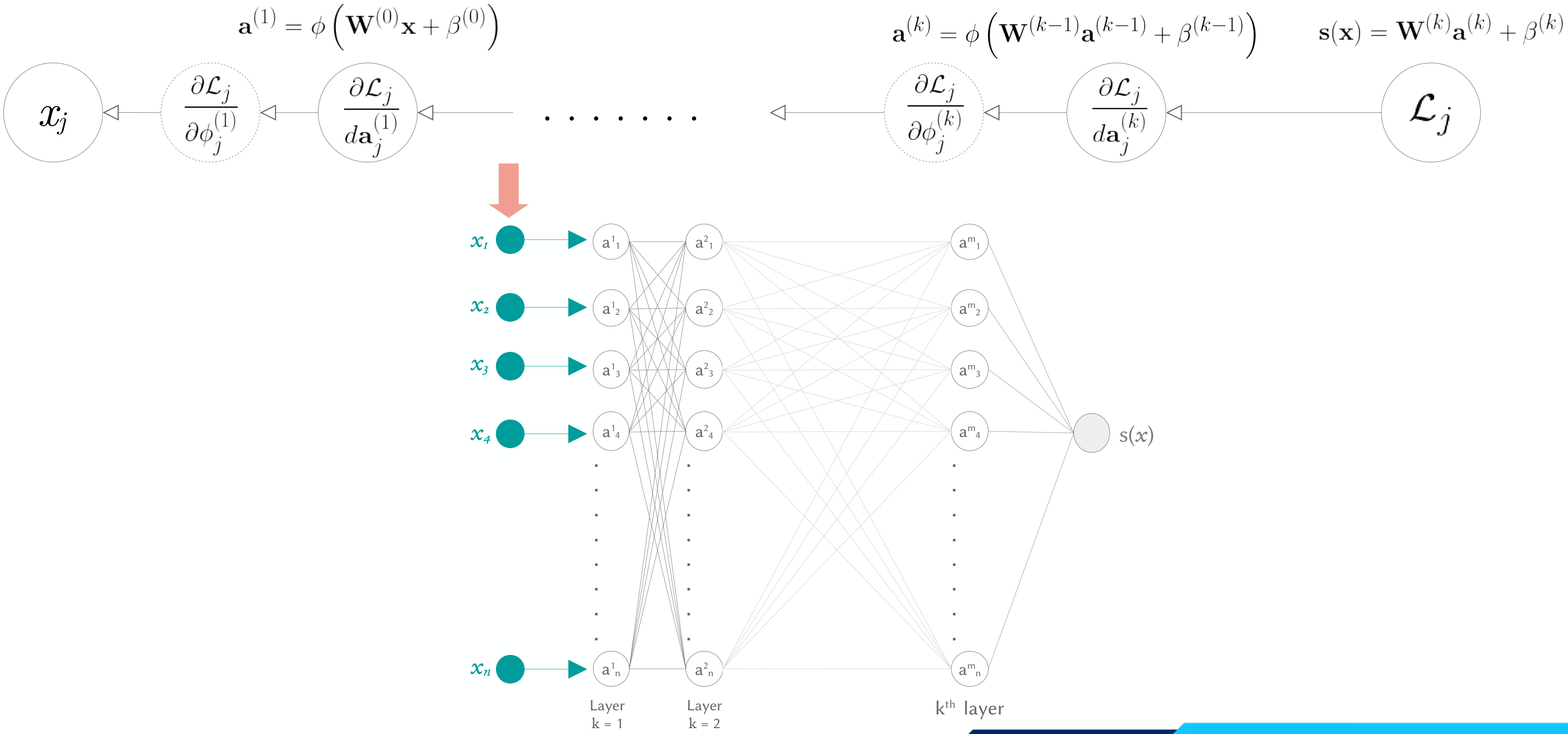
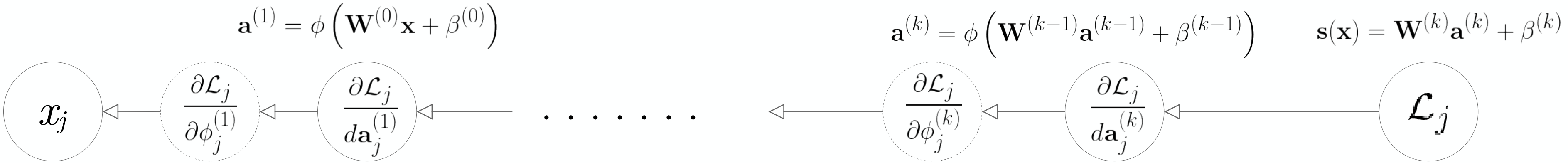


Backwards Propagation – Optimisation Algorithm



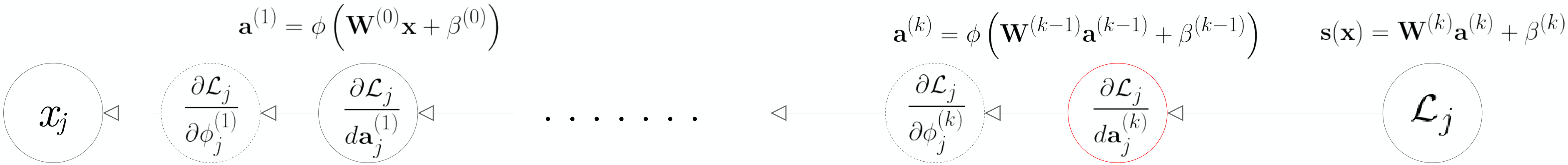
Backwards Propagation – Optimisation Algorithm



- **Chain rule** used to decompose the differential behaviour of the loss $\mathcal{L}$ per-layer (intermediate) variables in reverse order:

$$\frac{\partial y}{\partial x^{(1)}} = \frac{\partial x^{(2)}}{\partial x^{(1)}} \frac{\partial x^{(3)}}{\partial x^{(2)}} \frac{\partial y}{\partial x^{(3)}}$$

Backwards Propagation – Optimisation Algorithm



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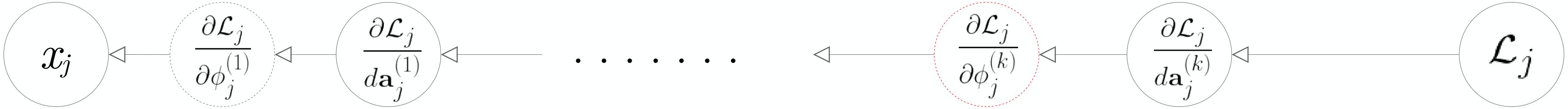

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$$\frac{\partial \mathcal{L}_j}{\partial \phi_j^{(k)}} = \frac{\partial \mathbf{a}_j^{(k)}}{\partial \phi^{(k)}} \frac{\partial \mathcal{L}_j}{\partial \mathbf{a}_j^{(k)}}$$

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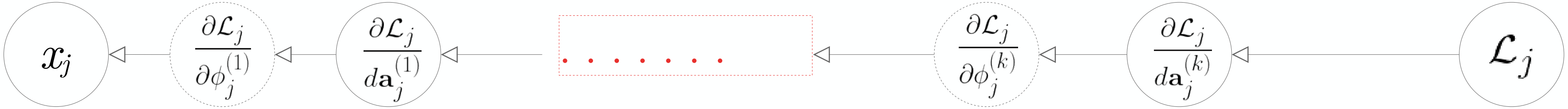

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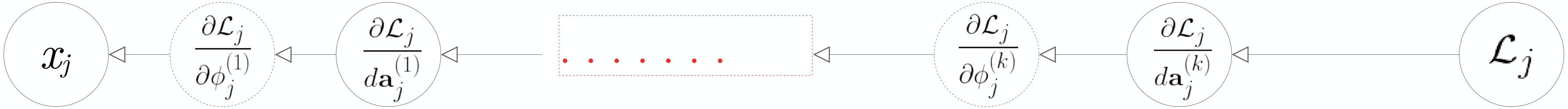

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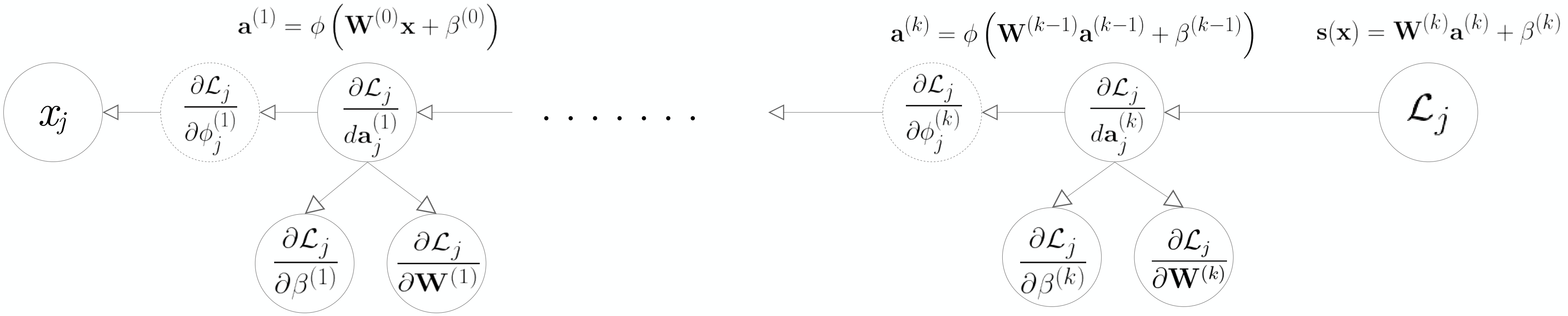
Backwards Propagation – Optimisation Algorithm



- **Chain rule** again used to decompose the differential behaviour of the loss $\mathcal{L}$ per-parameter $\Phi = \{W, \beta\}$:

$$\frac{\partial \mathcal{L}_j}{\partial \mathbf{W}_j^{(k)}} = \frac{\partial \mathbf{a}_j^{(k)}}{\partial \mathbf{W}^{(k)}} \frac{\partial \mathcal{L}_j}{\partial \mathbf{a}_j^{(k)}}$$

$$\frac{\partial \mathcal{L}_j}{\partial \beta_j^{(k)}} = \frac{\partial \mathbf{a}_j^{(k)}}{\partial \beta^{(k)}} \frac{\partial \mathcal{L}_j}{\partial \mathbf{a}_j^{(k)}}$$

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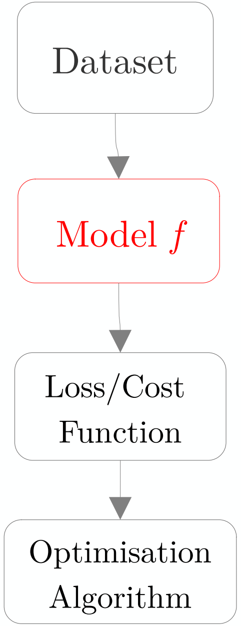
Recap

General recipe for *most* ML algorithms or learning processes:



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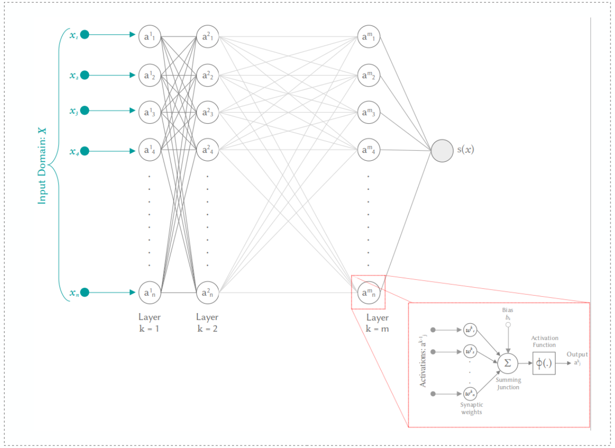
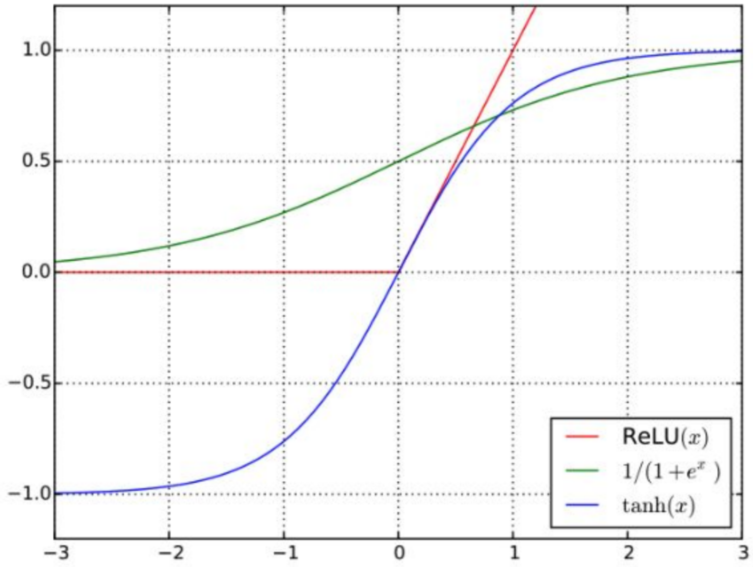


Activation Functions



- **Choice** of ϕ activation functions is pathological
- Decisions based on an array of factors
- The most common is the concept of **vanishing gradients**:

$$\frac{\partial \mathcal{L}_j}{\partial \mathbf{W}_j^{(k-2)}} = \frac{\partial \mathbf{a}_j^{(k-2)}}{\partial \mathbf{W}_j^{(k-2)}} \left(\underbrace{\frac{\partial \phi_j^{(k-1)}}{\partial \mathbf{a}_j^{(k-2)}}} \frac{\partial \mathbf{a}_j^{(k-1)}}{\partial \phi^{(k-1)}} \underbrace{\frac{\partial \phi_j^{(k)}}{\partial \mathbf{a}_j^{(k-1)}}} \frac{\partial \mathbf{a}_j^{(k)}}{\partial \phi^{(k)}} \frac{\partial \mathcal{L}_j}{\partial \mathbf{a}_j^{(k)}} \right)$$

Sigmoid	ReLU	Sigmoid	ReLU
$\leq 1/4$	≤ 1	$\leq 1/4$	≤ 1

Classification – Discrete Value Predictions

- **Task:** Classify using a dataset drawn from a joint distribution $p(x,y)$:

  Features $\boldsymbol{x} \in \mathbb{R}^n$

  Labels $\boldsymbol{y} \in \mathbb{R}$

- **Goal** is to predict y given an instance of x: $p(y=1|\mathbf{x}) = \dfrac{p(\mathbf{x}|y)p(y=1)}{p(\mathbf{x})}$

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$$= \frac{p(\mathbf{x}|y)p(y=1)}{p(\mathbf{x}|y=0)p(y=0) + p(\mathbf{x}|y=1)p(y=1)}$$

$$= \frac{1}{1 + \exp\left(\log\left(\frac{p(\mathbf{x}|y=0)p(y=0)}{p(\mathbf{x}|y=1)p(y=1)}\right)\right)}$$

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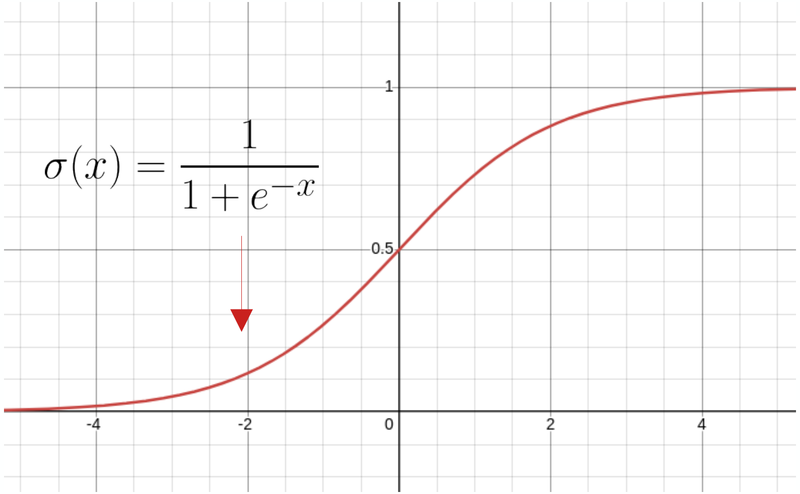

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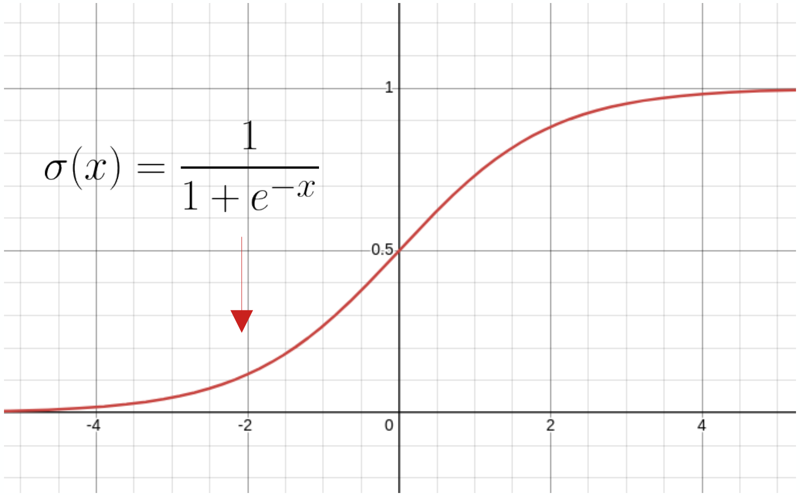

Log-Likelihood Ratio

$$p(y=1|\mathbf{x}) = \sigma\left(\log\left(\frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=0)}\right) + \log\left(\frac{p(y=1)}{p(y=0)}\right)\right)$$

Class Marginal
(does not depend on x)

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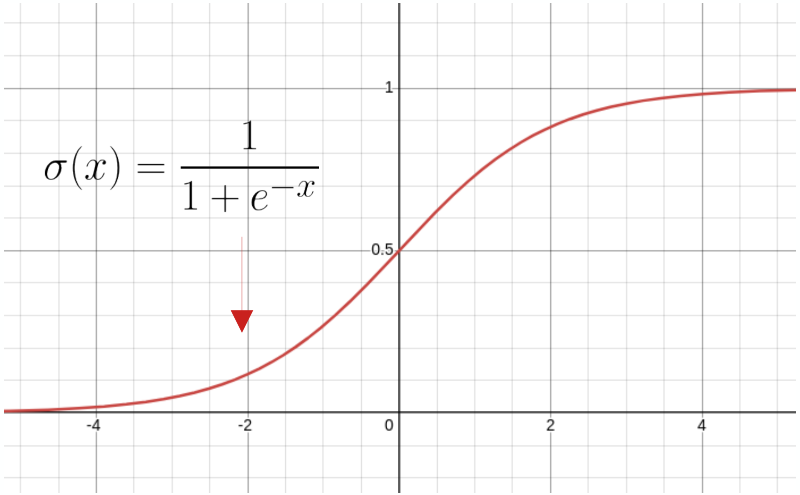
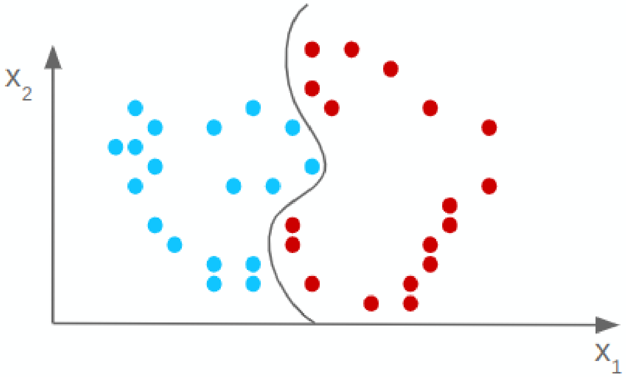


$$\sigma(x) = \frac{1}{1+e^{-x}}$$

The sigmoid converts the distance from a normal regression problem to a probabilistic decision boundary



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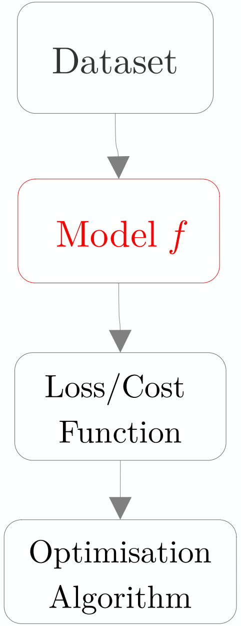

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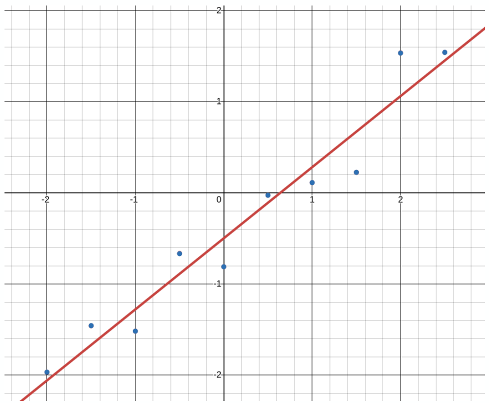


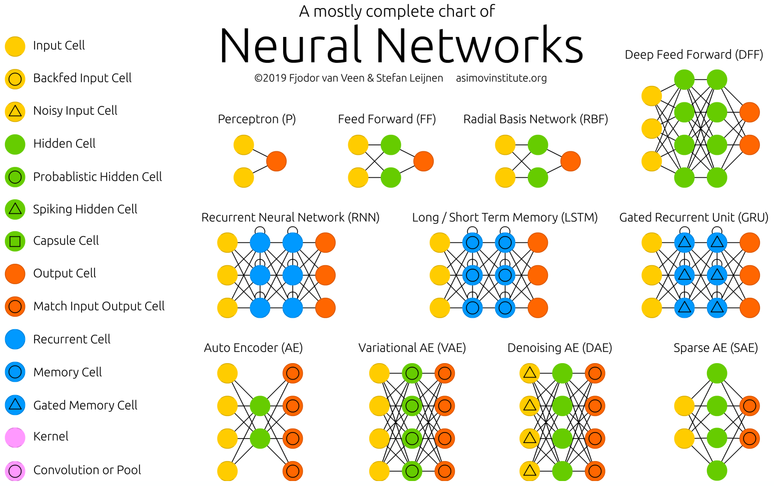
Linear Regression Example

Neural Zoo

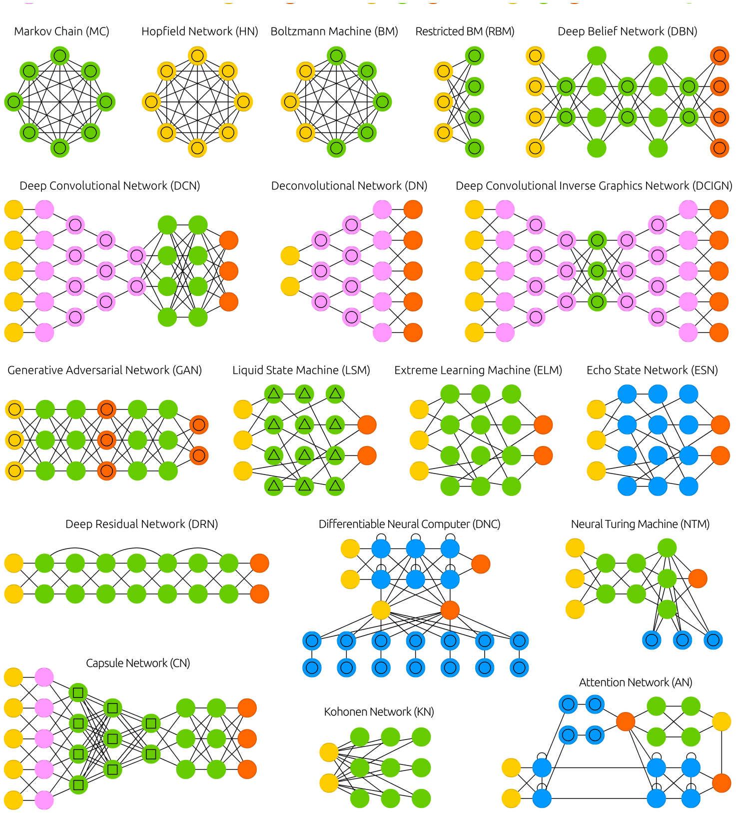
Diversity of Neural Networks

- **Ever growing** number of fundamental building blocks to neural based systems

- **No universally best block** for all uses cases, the various building blocks have different strengths and weaknesses



Source: link



Neural Zoo
Convolutional Neural Networks

Convolutional Neural Network

- **Extract** relevant **features** from a high dimensional input domain space given by the pixel space of an image of height and width **H** × **W** → $x \in \mathbb{R}^{H \times W}$

- **Salient features** ~ e.g. the lines of contrast between the foreground and the background

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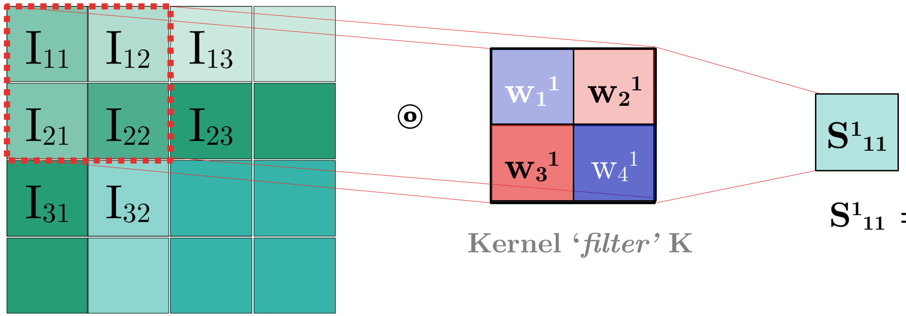
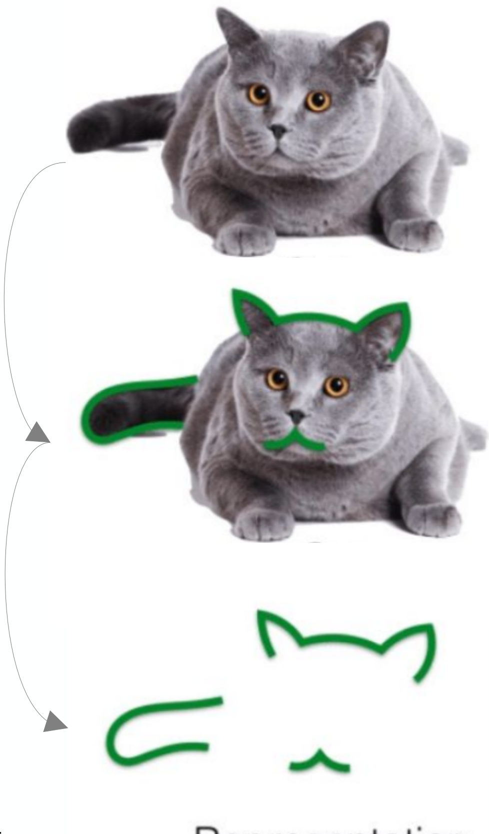
- **Salient features** ~ e.g. the lines of contrast between the foreground and the background

- The key building block is the **kernel filter:**

Image



$$S^1_{11} = w_1^1 I_{11} + w_2^1 I_{12} + w_3^1 I_{21} + w_4^1 I_{22}$$



Convolutional Neural Network

- **Extract** relevant **features** from a high dimensional input domain space given by the pixel space of an image of height and width **H** × **W** → $x \in \mathbb{R}^{H\times W}$

- **Salient features** ~ e.g. the lines of contrast between the foreground and the background

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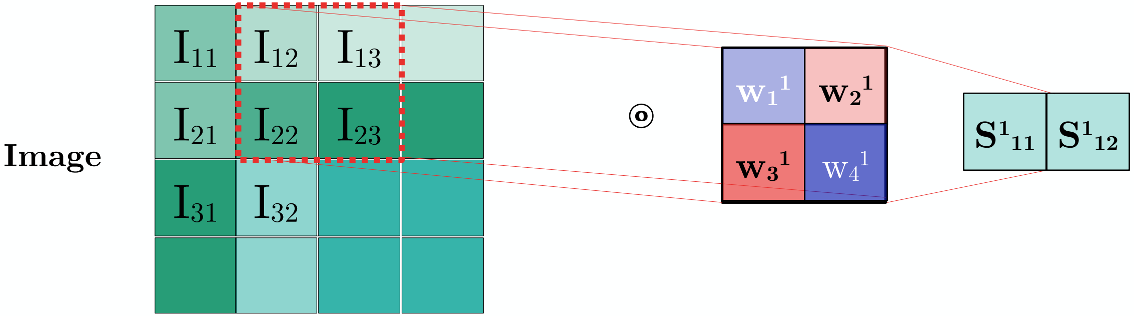

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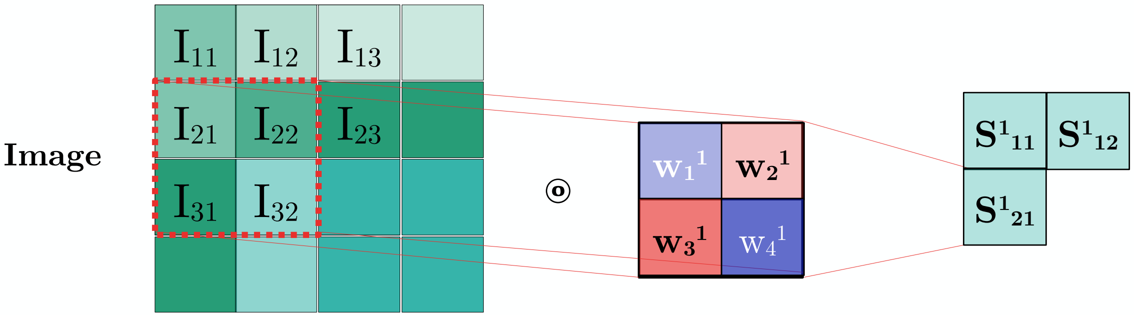

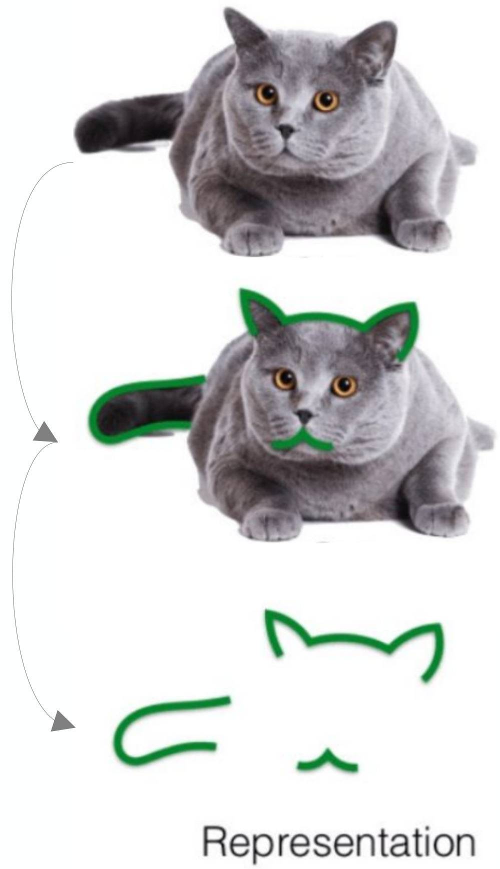

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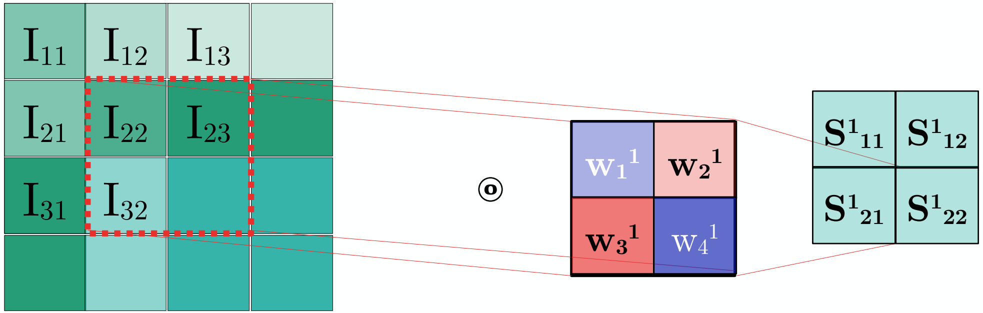


Convolutional Neural Network

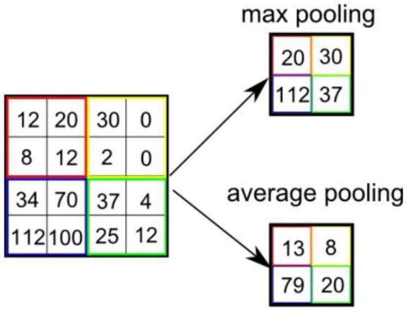
- **Formally** the kernel convolution operation:

$$S(i,j) = (I * K)(i,j) = \sum_m \sum_n I(m,n)K(i-m, j-n)$$

- **Salient feature map 'S' is by default smaller:**

$$\mathbf{S} \in \mathbb{R}^{(H-K+2P/S+1)\times(W—K+2P/S+1)}$$

- **Compressing** image size further to reduce input dimension by **max/average pooling**



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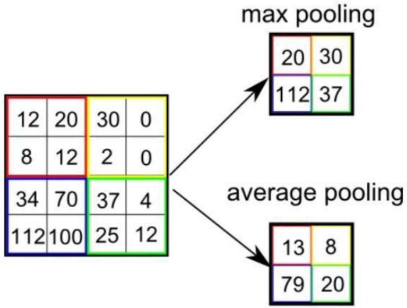

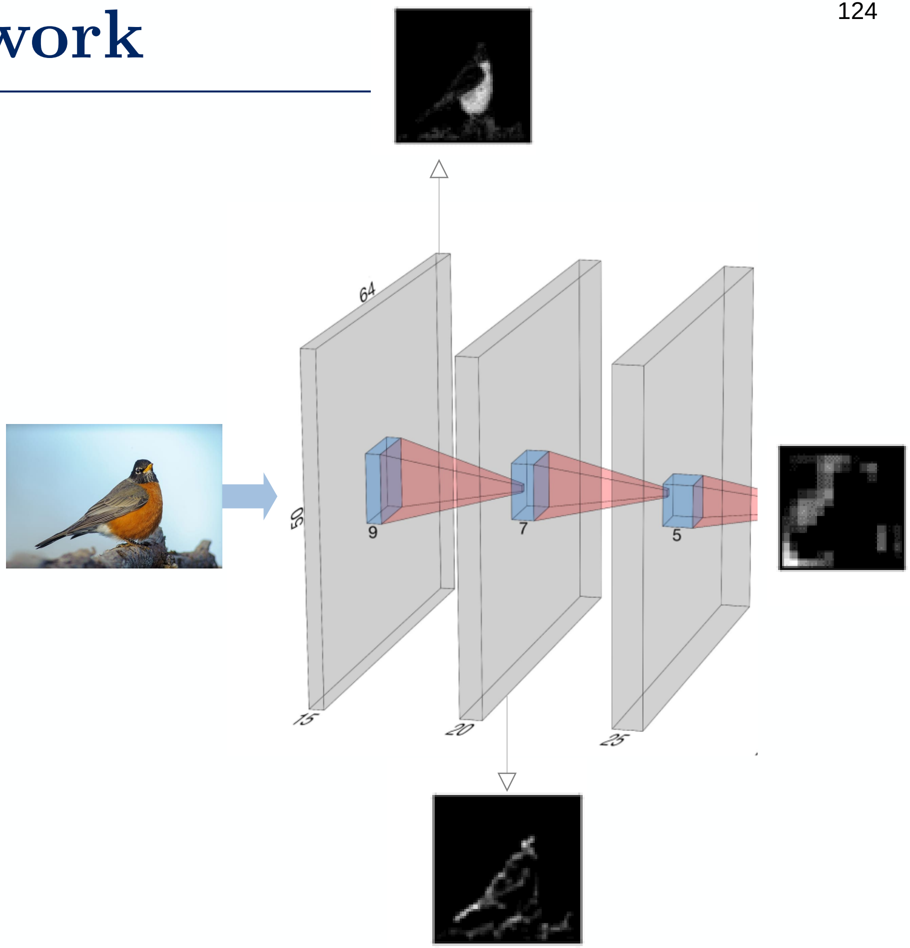

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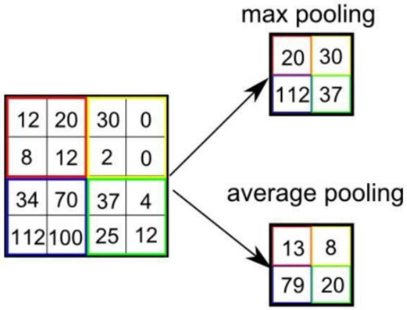
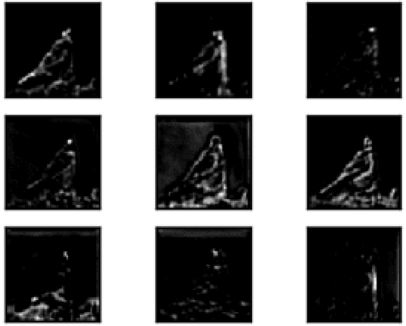


CNN Layer 1

x6 Kernels

CNN Layer 2

x6 Kernels



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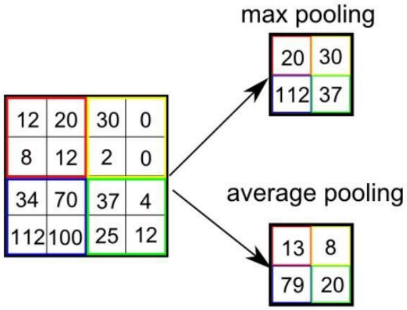
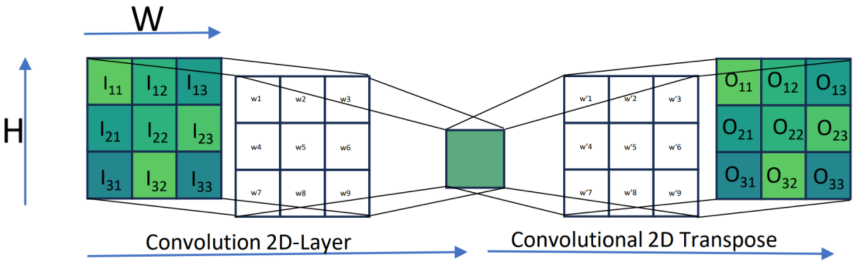


- The **inverse transpose operation** expands the image:



Neural Zoo
Transformers

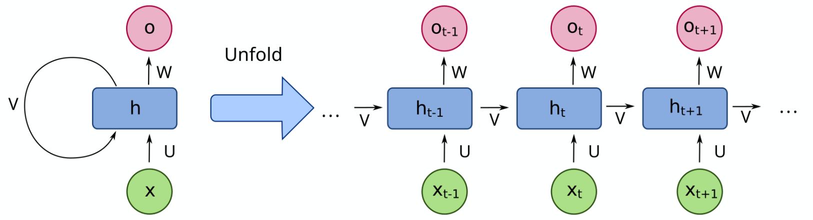
Transformers

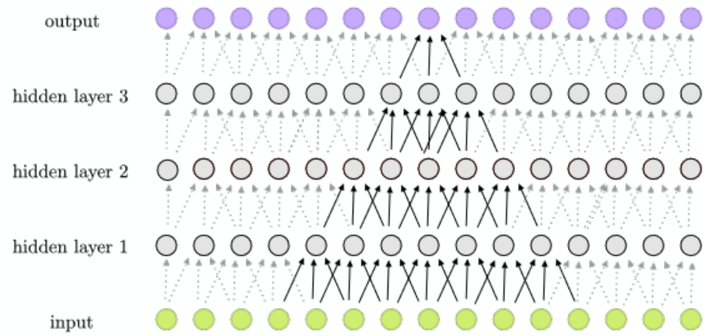
- **Before Transformers:**
  - **Recurrent Neural Networks:**

    Sequential models utilise recurrent connections, in which the output of the network is passed from time step t to t+1 via a recurrent unit – great sequences

  - **Convolution Neural Networks:**

    Model that utilises kernel filters to learn 'salient' features by convoluting nearby activity into increasingly abstract features – great for local information extraction in sequences





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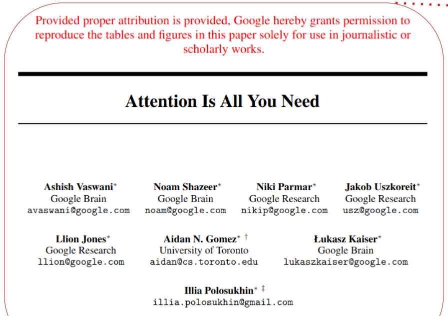
- **Transformers:**
  - Introduced **attention mechanisms**
  - Provides information about all positions **simultaneously**
  - Great for **sequences,** and geometrical data such as **images**



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Attention Is All You Need

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Source: arXiv:1706.03762

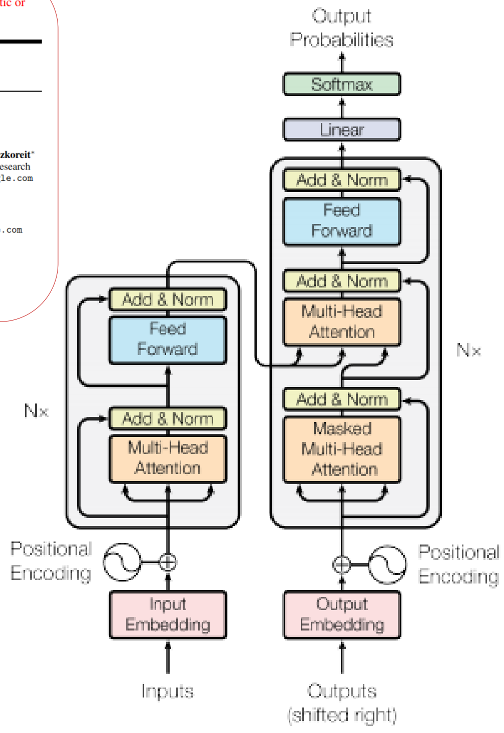

Figure 1: The Transformer - model architecture.

Context Matters – Global Attention

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$p(x_i|\mathcal{C} = \text{'Small cute animal with wide eyes'})$

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The distribution of pixel values can be generated to reflect a conditional probability:

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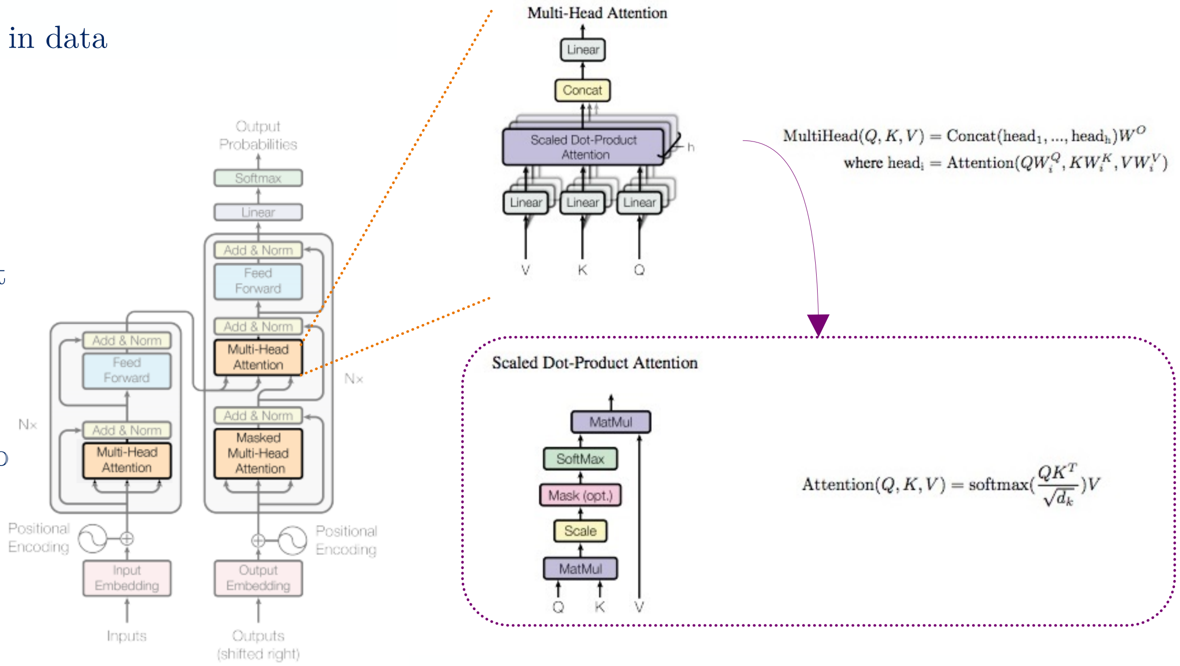
But what we want is each pixel to be dependent on the context and the rest of the pixel values:

$$p(x_i|\mathcal{C} = \text{'Small cute...'}, \sum_{j \neq i}^{H \times W} x_j)$$

Transformers – Scaled dot-product attention

- **Advantages of Transformers (physics focus):**
  - Handle variable length data
  - Capture **long-range dependencies** in data
  - Permutation/order invariant
  - Highliy parallelisable

- **Attention Mechanism:**
  - The success of transformers resides at *first order* in the introduction of the attention mechanism
  - Understanding attention needs you to understand the idea of:
    - **vector embeddings**
    - **attention**



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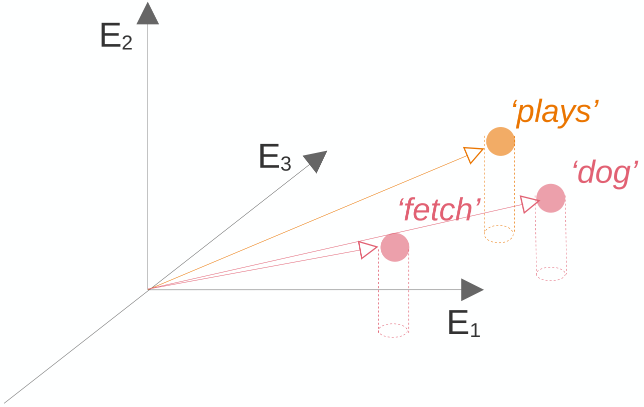
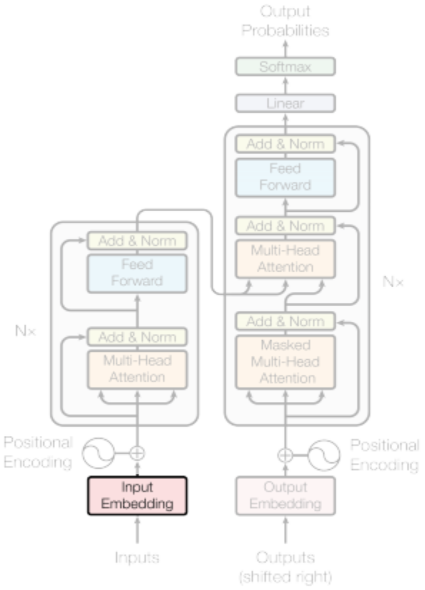
Transformers – Vector Embeddings

- **Transformers act on vectors:**
  - **Tokenisation+embedding** turns each element of the sequence into a vector that resides in a vector space:

$x_i =$ dog | plays | fetch → Embedding →

$$\begin{pmatrix} +.0.36 & +0.63 & -0.23 \\ +.0.21 & +0.47 & +0.18 \\ +.0.25 & +0.92 & -0.47 \end{pmatrix}^T$$





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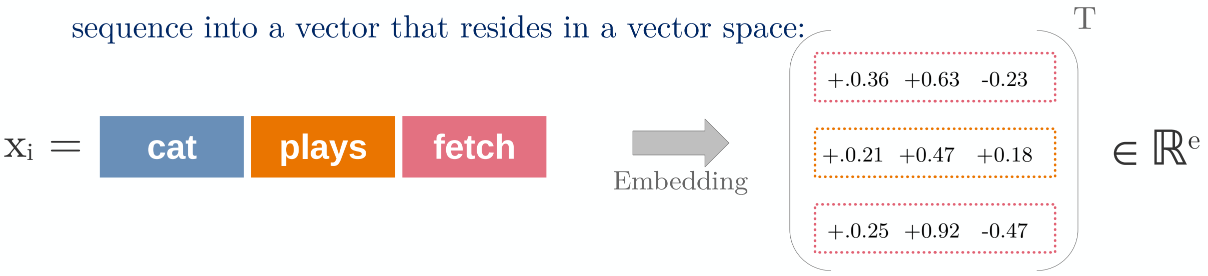

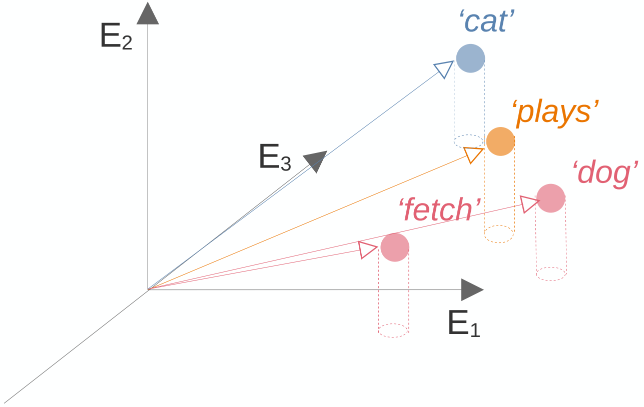

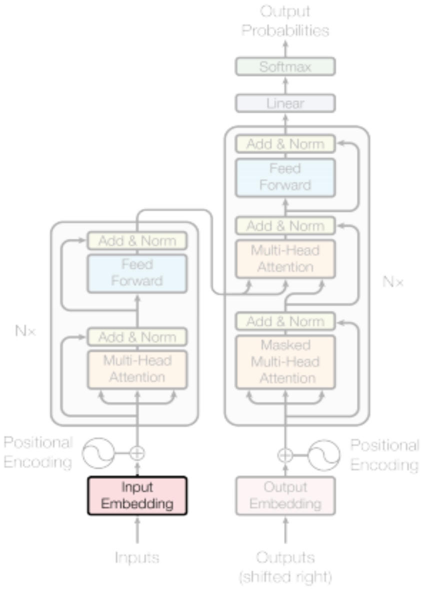

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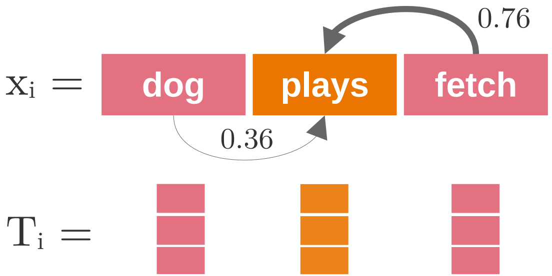
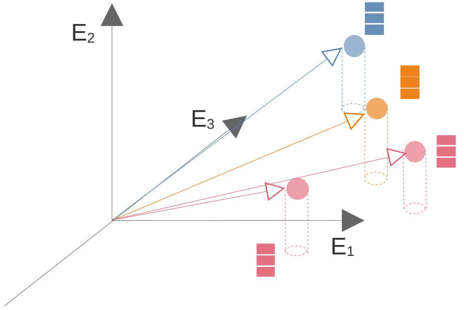
Transformers – Attention

- **Attention = Dynamic flow of information**
  - Each **embedded token** stores which token matters and by how much

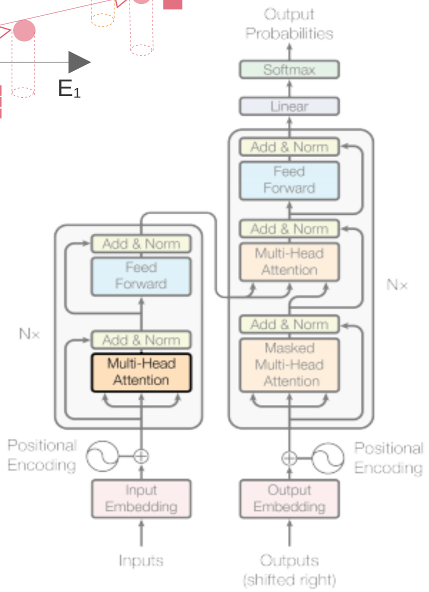




  - **Scaled-dot product** attention is one type of attention that achieves this goal:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

  - Three key ingredients:
    - **Query (Q)** : What am I looking for?
    - **Key (K)** : What do I have to offer?
    - **Value (V)** : What do I share if picked?



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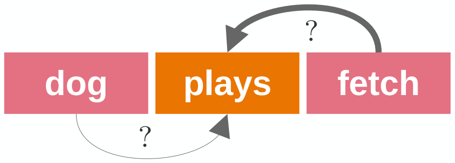
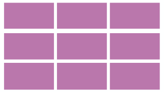
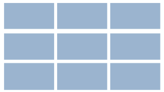
Transformers – Visualising Attention

- **Lets see how this works for a simple case:**

$x_i =$ 

- **1) Define scaled-dot product** attention weights for optimisation:
  - $\mathbf{W_Q}$ **:** Matrix of weights for queries, shape = [n, e] 
  - $\mathbf{W_K}$ **:** Matrix of weights for keys, shape = [n, e] 
  - $\mathbf{W_V}$ **:** Matrix of weights for values, shape = [n, e] 

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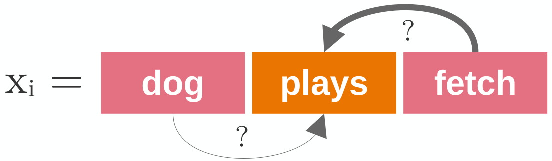
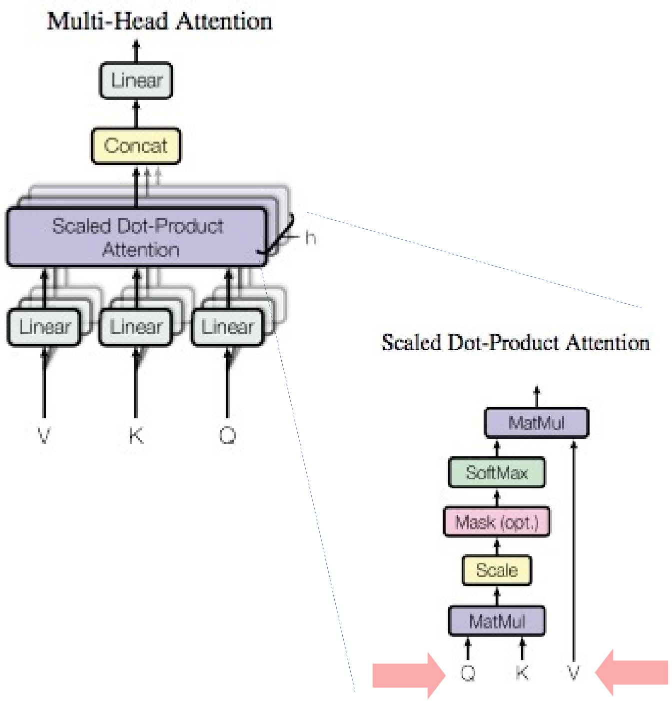


- **2)** Compute the query, key and value triplet **(Q,K,V)** for **'plays'**
  - $\mathbf{Q_{plays}}$: $W_Q \cdot T_p$ = · = [1,e]
  - $\mathbf{K_{d(f)}}$: $W_K \cdot T_{d(f)}$ = · = [1,e]
  - $\mathbf{V_{d(f)}}$: $W_V \cdot T_{d(f)}$ = · = [1,e]

$$\text{MultiHead}(Q,K,V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W^O$$
$$\text{where head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$



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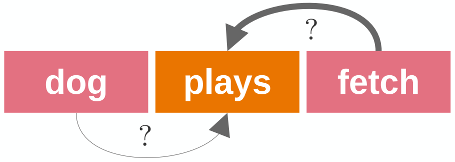
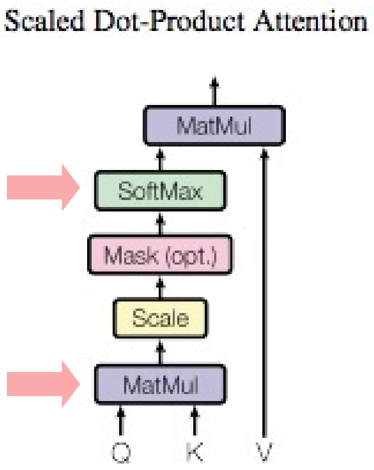
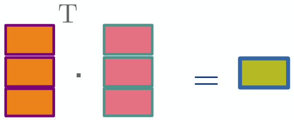
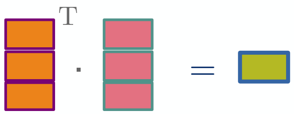
$x_i =$ 



- **2)** Compute the **similarity** between **'dog(fetch)'** to ''**play**'
  - $\mathbf{S}_{\textbf{plays-dog}}$ **:** $Q_{plays} \,.\, K_d =$  $=$ [1,1]
  - $\mathbf{S}_{\textbf{plays-fetch}}$ **:** $Q_{plays} \,.\, K_f =$  $=$ [1,1]

- **3)** Convert to **Similarity** to **'scaled weights'**:
  - $\mathbf{a}^{\mathbf{p}}_{\mathbf{d(f)}}$ **:** $\sigma(\, S_{plays\text{-}dog(fetch)} \,) = \sigma($  $) =$  Softmax forces values to be in range [0,1]

Transformers – Visualising Attention

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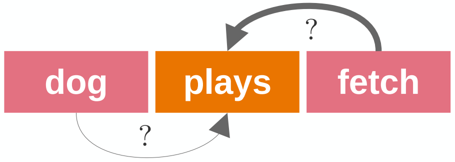
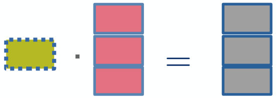
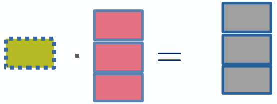
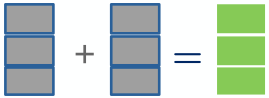
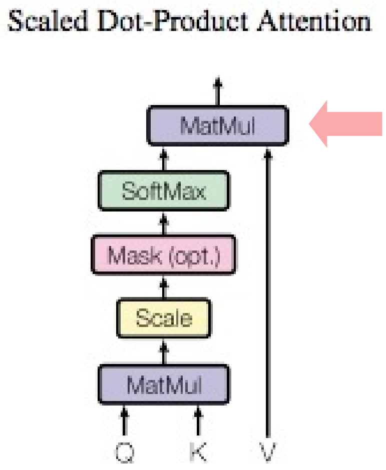
$x_i =$ 

- **4)** Form the context of ‘**plays**’ relative to ‘**dog**’ & ‘**fetch**’:
  - $\mathbf{C_{plays\text{-}dog}}$ **:** $a^{p}_{d} \,.\, V_d \;=$  [1,e]
  - $\mathbf{C_{plays\text{-}fetch}}$ **:** $a^{p}_{f} \,.\, V_f \;=$  [1,e]
- 5) What is the total context of ‘**plays**’?
  - $\mathbf{C_{plays}}$: $\mathbf{C_{plays\text{-}dog}} + \mathbf{C_{plays\text{-}fetch}} =$  [1,e]



Transformers – Visualising Attention

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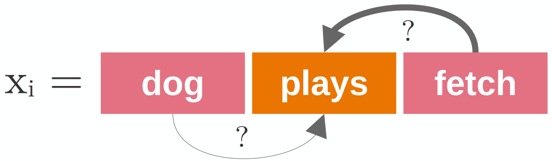
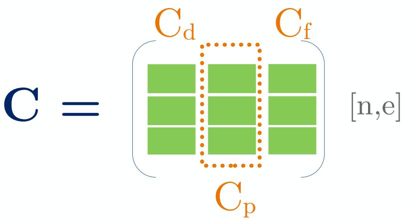
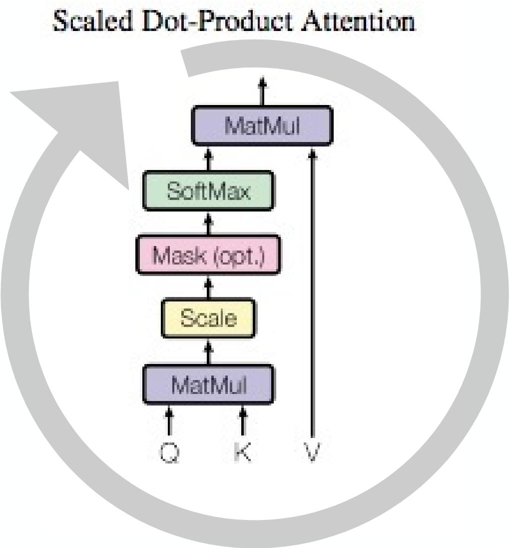


- **6)** Repeat now for **'dog'** and **'fetch'**:





Transformers – Visualising Attention

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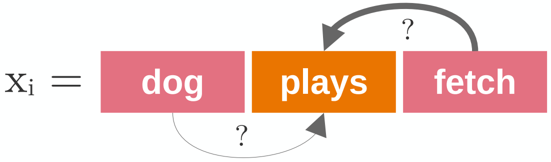

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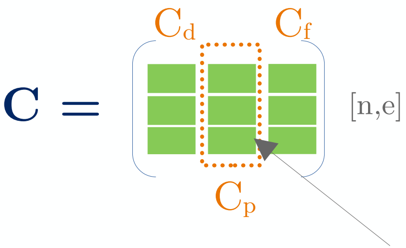
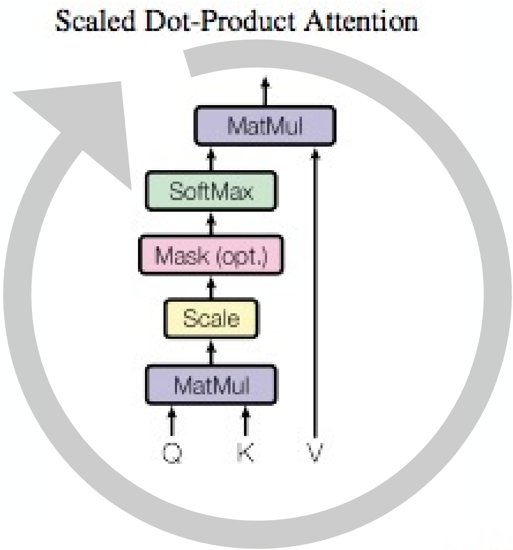


What is the context of all embedding vectors to the word 'play'?



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Transformers – Visualising Attention

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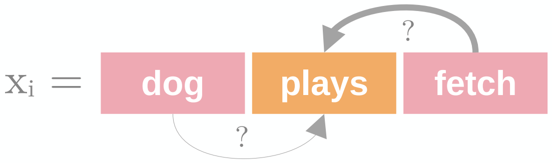

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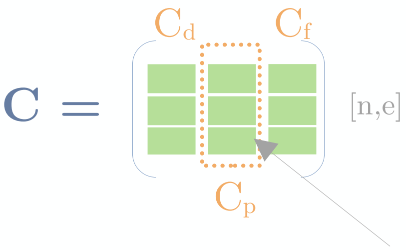

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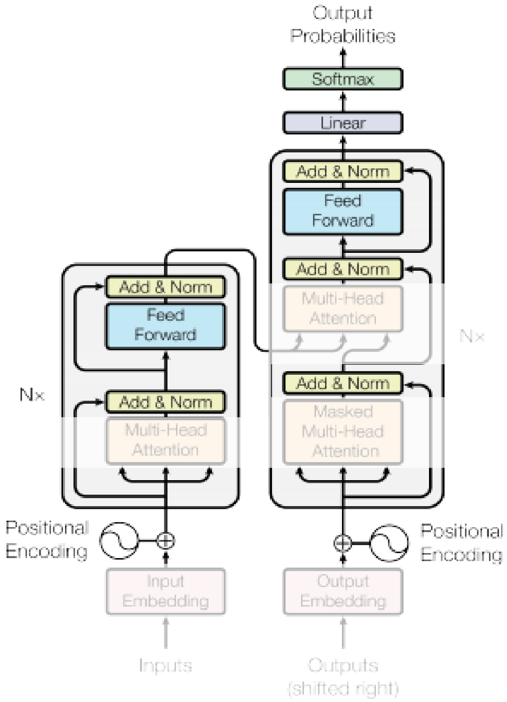

Figure 1: The Transformer - model architecture.

The rest of the transformer is actually quite simple
– just MLPs and adding/normalisation

The End

Thank you!

Resources

- **Books:**

  [1] I.Goodfellow, Y.Bengio, and A.Courville, *'Deep Learning'*, MIT Press, 2016, http://www.deeplearningbook.org

  [2] Simon J.D. Prince, '*Understanding Deep Learning'*, MIT Press, 2023, http://udlbook.com

  [3] Kevin P. Murphy, "Probabilistic Machine Learning: An introduction", MIT Press, 2022, probml.ai

- **Lectures:**

  [1] ATLAS-D 2023, F.Meloni, https://indico.cern.ch/event/1263122/

  [2] G.Louppe, Info8010 Deep Learning, 2024, https://github.com/glouppe/info8010-deep-learning

- **Misc.** :

  [1] Kaare Petersen, Michael Pedersen, '*Matrix Cookbook*', 2012, https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

Backup

Point Estimators: Technicality of continuous variables

- **Covariance:** Linear correlation between two variables:

$$Cov(f(x), g(y)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])(g(y) - \mathbb{E}[g(y)])\right]$$

- **Deterministically Correlated Random Variables:**
  → Two random variables X & Y, such that $y = g(x)$:

$$p_x(x) = p_y(g(x)) \left| \frac{\partial g(x)}{\partial x} \right|$$

  → In higher dimensions $\mathbf{x}$ & $\mathbf{y}$, for $\mathbf{x} = g(\mathbf{y})$:

$$p_x(\mathbf{x}) = p_y(g(\mathbf{x})) \left| \det \left(\frac{\partial g(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

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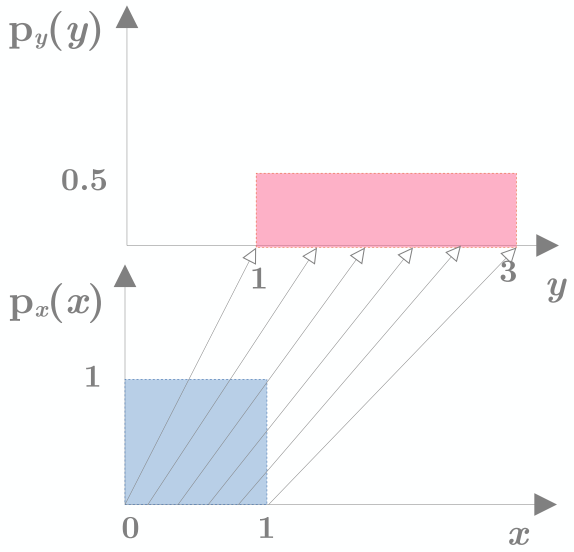

Estimator Properties

- **Point Estimator, or statistic**, is any function of the data that infers from the data some parameter of interest θ:

$$\hat{\theta} = g(\{x\}_m)$$

- **Bias** of an estimator is given by:

$$\text{bias}(\hat{\theta}) = \mathbb{E}(\hat{\theta}) - \theta$$

- **Variance** of an estimator:

$$\text{Var}(\hat{\theta})$$

- **Example – Gaussian:**
Sample $\{x\}_m$ generated by a Gaussian *pdf*:

$$\hat{\sigma}^2 = \frac{1}{m}\sum\left[(x_i - \hat{\mu})^2\right] \longleftarrow p(x_i|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{1}{2}\frac{(x_i-\mu)^2}{\sigma^2}\right]$$

→ Bias calculation:

$$\text{bias}(\hat{\sigma}^2) = \underbrace{\mathbb{E}(\hat{\sigma}^2)} - \sigma^2 = -\frac{\sigma^2}{m}$$

$$\mathbb{E}(\hat{\sigma}^2) = \mathbb{E}\left[\frac{1}{m}\sum(x_i - \hat{\mu})^2\right] = \frac{m-1}{m}\sigma^2$$

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$\rightarrow$ Bias calculation:

$$\text{bias}(\hat{\sigma}^2) = \mathbb{E}(\hat{\sigma^2}) - \sigma^2 = 0$$

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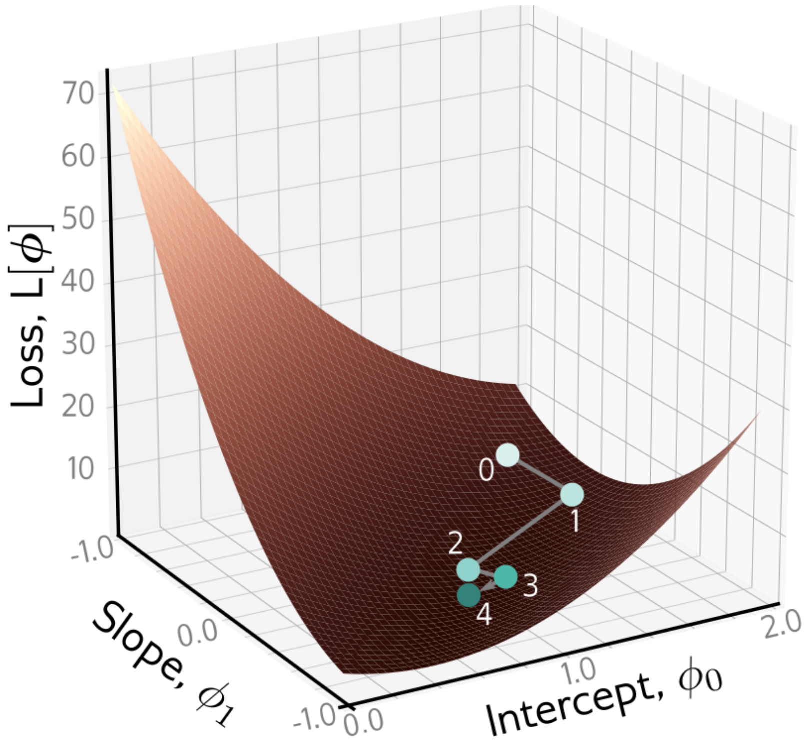
$$\text{Var}(\hat{\mu}) = \text{Var}(\frac{1}{m}\sum_i^m x_i) = \mathbb{E}\left[\left(\frac{1}{m}(\sum_i^m x_i - \mathbb{E}(\sum_i^m x_i))\right)^2\right]$$

$$= \frac{1}{m^2}\sum_i^m \text{Var}(x_i) = \frac{\sigma^2}{m^2}$$

Gradient Descent



- Optimising the model f is achieved by minimising the **loss/cost function**:

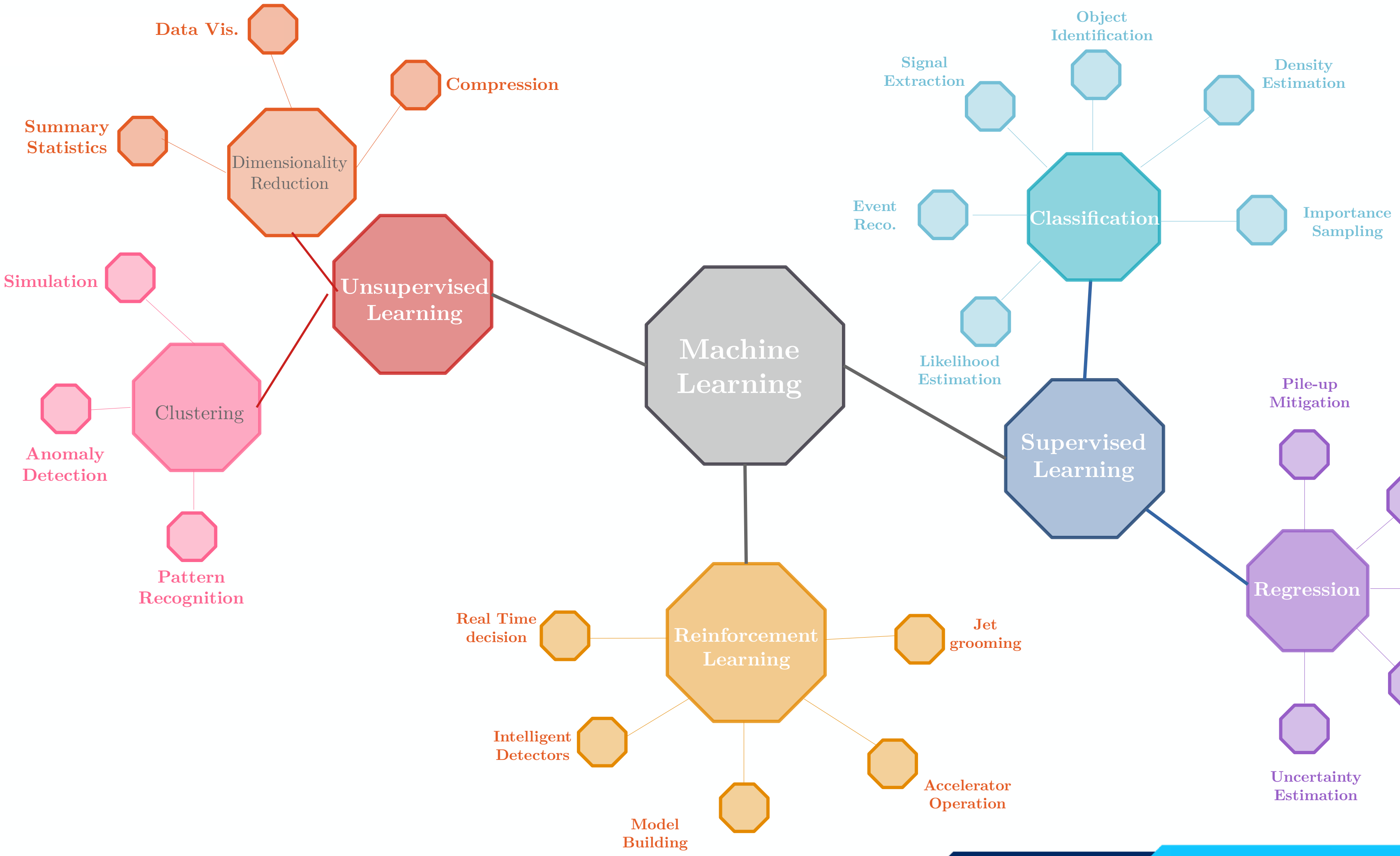
$$\hat{\Phi} = \arg\min \left[\mathcal{L}(f(\mathbf{x}|\Phi), \mathbf{x}) \right]$$

- **Gradient descent** has primarily two steps:
  1) Calculate gradients:

$$\frac{\partial \mathcal{L}}{\partial \Phi} = \begin{bmatrix} \frac{d\mathcal{L}}{\partial \phi_0} \\ \cdots \\ \frac{d\mathcal{L}}{\partial \phi_h} \end{bmatrix}$$

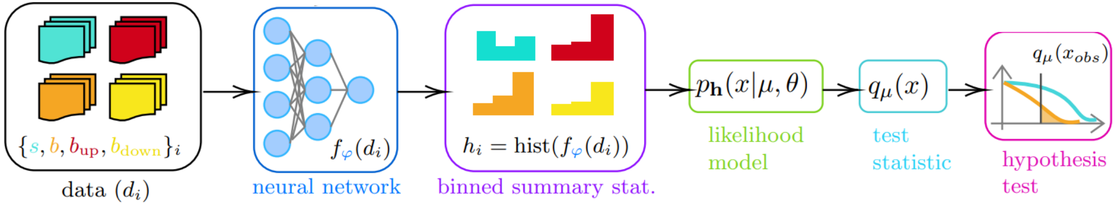
  2) Update the parameters in direction that minimises loss:

$$\phi_i \leftarrow \phi_i - \alpha \frac{\partial \mathcal{L}}{\partial \phi_i}$$


Machine Learning
Unsupervised Learning
Dimensionality Reduction
Data Vis.
Compression
Summary Statistics
Clustering
Simulation
Anomaly Detection
Pattern Recognition
Supervised Learning
Classification
Object Identification
Signal Extraction
Density Estimation
Event Reco.
Importance Sampling
Likelihood Estimation
Regression
Pile-up Mitigation
Calibration
Function Approx.
Parameter Estimation
Uncertainty Estimation
Reinforcement Learning
Real Time decision
Jet grooming
Intelligent Detectors
Model Building
Accelerator Operation

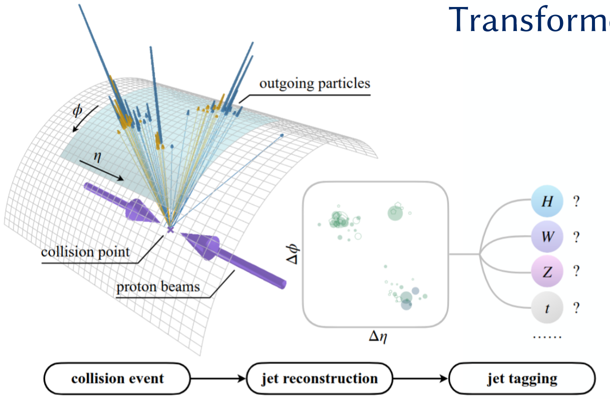
High Energy Physics – ML Developments

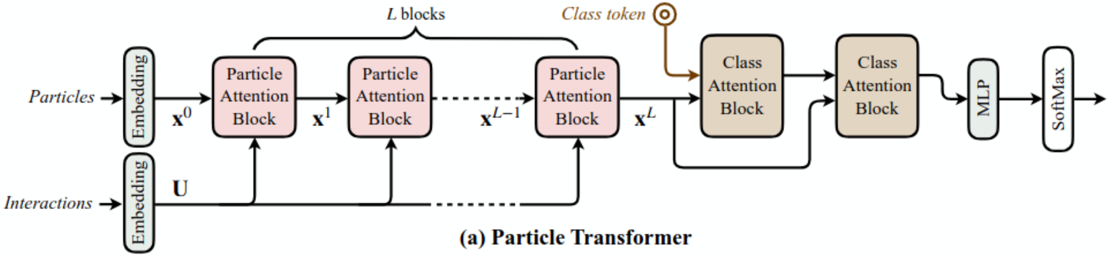
→ Checkout the HEP Machine Learning Living Review



Particle Transformer - arXiv:2202.03772

Transformer model for tagging jets at the LHC





(a) Particle Transformer

Probability Triplet

Can likely skip

Continuous Probability

- **Absolute continuous probability** is the infinitesimal sum[1] over the **probability density function** $p : \mathbb{R} \to [0, \infty]$:

$$P(X \in A) = \int_A p(x)dx$$

- **Marginal probability** density:

$$p(x) = \int p(x, y)dy$$

- **Conditional probability** density:

$$p(y|x) = \frac{p(x, y)}{p(x)}$$

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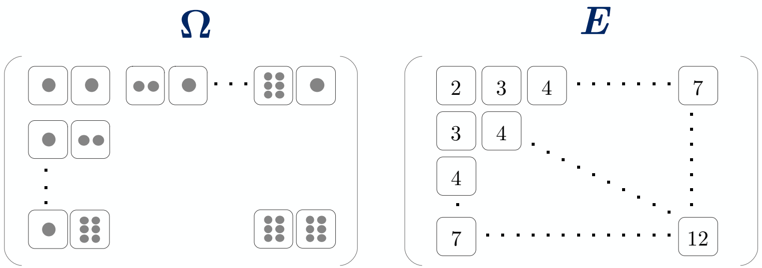

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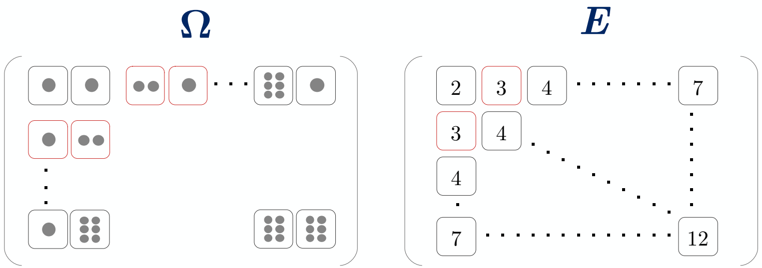

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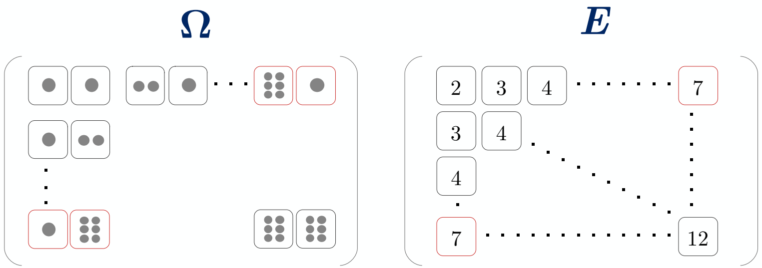

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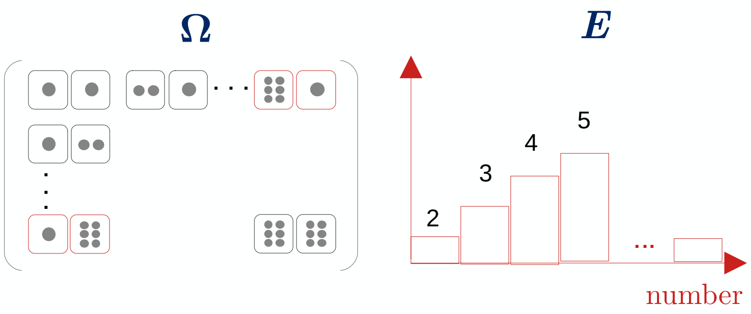

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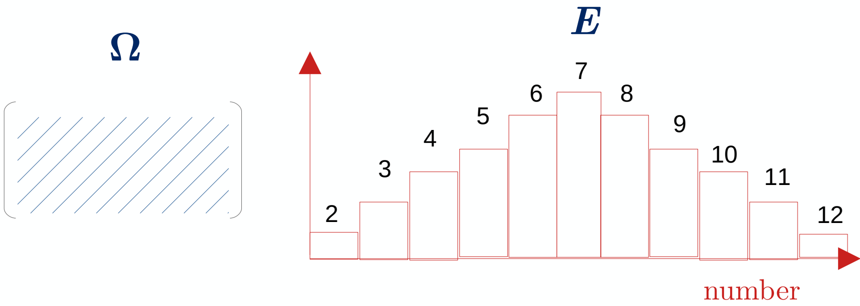

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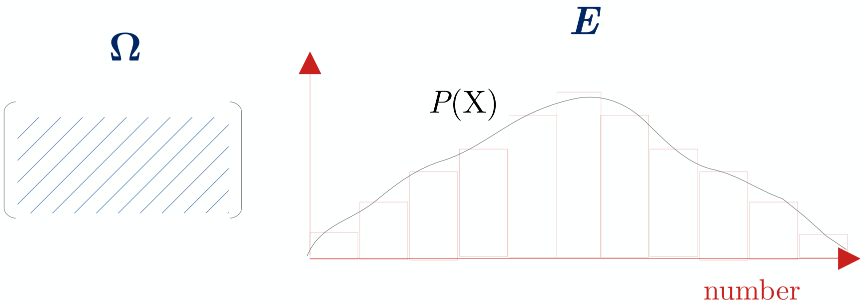

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- **(Non-)Conditional Independence:**

  Two random variables are independent if:

$$p(\mathbf{x} = x, \mathbf{y} = y) = p(\mathbf{x} = x)p(\mathbf{y} = y)$$

$$\forall x \in \mathbf{x},\ \forall y \in \mathbf{y}$$

[1] *kind of…see uncountable sets*

Point Estimators: Expectation, bias, variance

- **Expectation:** Expected value of a function of random variables

$$\mathbb{E}_{x\sim p}[f(x)] = \int p(x)f(x)dx$$

- **Variance:** Variation of samples from a random variable:

$$Var(f(x)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])^2\right]$$

- **Covariance:** Linear correlation between two variables:

$$Cov(f(x), g(y)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])(g(y) - \mathbb{E}[g(y)])\right]$$