Mathematics for Machine Learning

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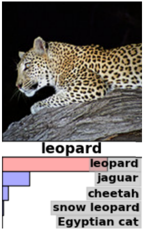
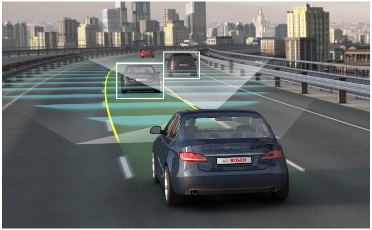
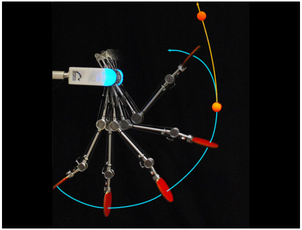
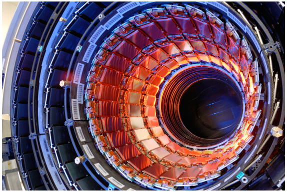
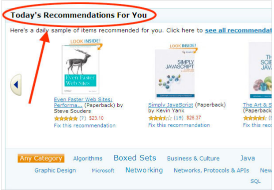
Applications of Machine Learning

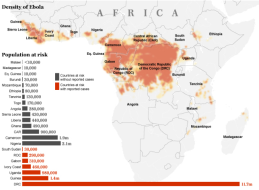




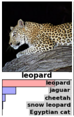


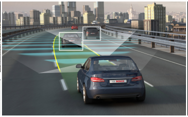
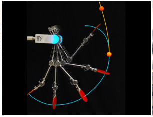
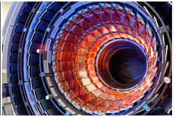
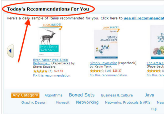


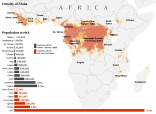




Mathematical Concepts in Machine Learning





- Linear algebra and matrix decomposition
- **Differentiation**
- Optimization
- **Integration**
- Probability theory and Bayesian inference
- Functional analysis

Outline

Overview

Introduction

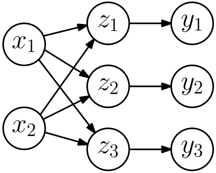
Differentiation

Integration

Feedforward Neural Network

$$\boldsymbol{y} = \sigma(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$$



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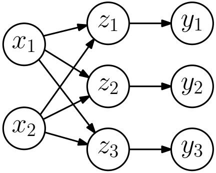

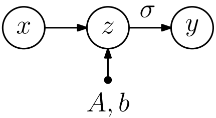

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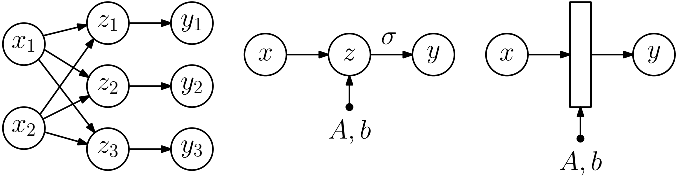

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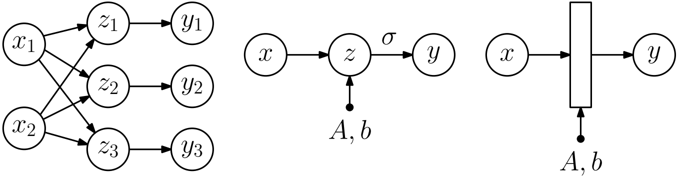

- Training a neural network means parameter optimization: Typically via some form of gradient descent
  ▶▶ **Challenge 1: Differentiation.** Compute gradients of a loss function with respect to neural network parameters $\boldsymbol{A}, \boldsymbol{b}$

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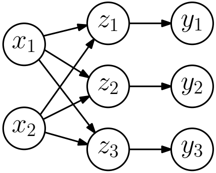
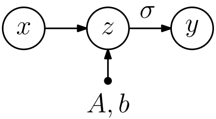
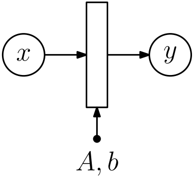


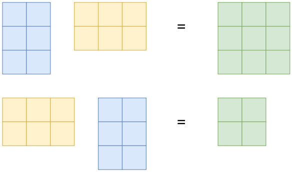




- Training a neural network means parameter optimization: Typically via some form of gradient descent
  ▶▶ **Challenge 1: Differentiation.** Compute gradients of a loss function with respect to neural network parameters $\boldsymbol{A}, \boldsymbol{b}$
- Computing statistics (e.g., means, variances) of predictions
  ▶▶ **Challenge 2: Integration.** Propagate uncertainty through a neural network

Background: Matrix Multiplication

- Matrix multiplication is not commutative, i.e., $\boldsymbol{AB} \neq \boldsymbol{BA}$



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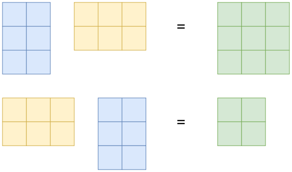

- Matrix multiplication is not commutative, i.e., $\boldsymbol{A}\boldsymbol{B} \neq \boldsymbol{B}\boldsymbol{A}$

- When multiplying matrices, the "neighboring" dimensions have to fit:

$$\underbrace{\boldsymbol{A}}_{n \times k} \underbrace{\boldsymbol{B}}_{k \times m} = \underbrace{\boldsymbol{C}}_{n \times m}$$

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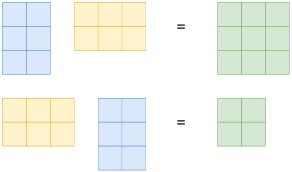

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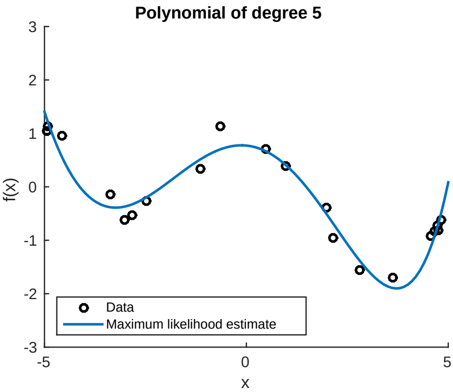
$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ `y = A.dot(x)`

$y_i = \sum_j A_{ij}x_j$ `y = np.einsum('ij, j', A, x)`

$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$ `C = A.dot(B)`

$C_{ij} = \sum_k A_{ik}B_{kj}$ `C = np.einsum('ik, kj', A, B)`

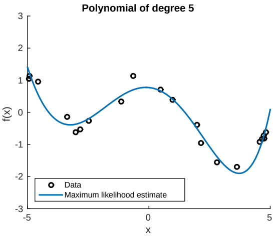
Curve Fitting (Regression) in Machine Learning (1)



- Setting: Given inputs $\boldsymbol{x}$, predict outputs/targets $\boldsymbol{y}$
- Model f that depends on parameters $\boldsymbol{\theta}$. Examples:
    - Linear model: $f(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{x}, \quad \boldsymbol{x}, \boldsymbol{\theta} \in \mathbb{R}^D$
    - Neural network: $f(\boldsymbol{x}, \boldsymbol{\theta}) = NN(\boldsymbol{x}, \boldsymbol{\theta})$

Curve Fitting (Regression) in Machine Learning (2)

- Training data, e.g., N pairs $(\boldsymbol{x}_i, y_i)$ of inputs $\boldsymbol{x}_i$ and observations y_i
- Training the model means finding parameters $\boldsymbol{\theta}^*$, such that $f(\boldsymbol{x}_i, \boldsymbol{\theta}^*) \approx y_i$



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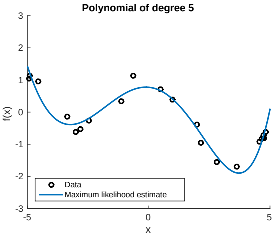


- Define a loss function, e.g., $\sum_{i=1}^{N}(y_i - f(\boldsymbol{x}_i, \boldsymbol{\theta}))^2$, which we want to optimize
- Typically: Optimization based on some form of gradient descent
  ▸▸ Differentiation required

Overview

Introduction

Differentiation

Integration

Differentiation: Outline

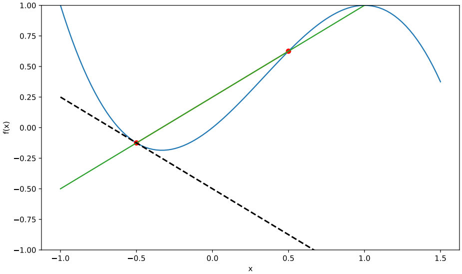
1. Scalar differentiation: $f : \mathbb{R} \to \mathbb{R}$
2. Multivariate case: $f : \mathbb{R}^N \to \mathbb{R}$
3. Vector fields: $f : \mathbb{R}^N \to \mathbb{R}^M$
4. General derivatives: $f : \mathbb{R}^{M \times N} \to \mathbb{R}^{P \times Q}$

Scalar Differentiation $f : \mathbb{R} \to \mathbb{R}$

- Derivative defined as the limit of the difference quotient

$$f'(x) = \frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

▶▶ Slope of the secant line through $f(x)$ and $f(x+h)$



Examples

$$
\begin{aligned}
f(x) &= x^n & f'(x) &= nx^{n-1} \\
f(x) &= \sin(x) & f'(x) &= \cos(x) \\
f(x) &= \tanh(x) & f'(x) &= 1 - \tanh^2(x) \\
f(x) &= \exp(x) & f'(x) &= \exp(x) \\
f(x) &= \log(x) & f'(x) &= \frac{1}{x}
\end{aligned}
$$

Rules

- Sum Rule

$$\big(f(x) + g(x)\big)' = f'(x) + g'(x) = \frac{df}{dx} + \frac{dg}{dx}$$

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- Chain Rule

$$(g \circ f)'(x) = \big(g(f(x))\big)' = g'(f(x))f'(x) = \frac{dg}{df}\frac{df}{dx}$$

Example: Chain Rule

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$$\begin{aligned} g(z) &= \tanh(z) \\ z &= f(x) = x^n \\ (g \circ f)'(x) &= \end{aligned}$$

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$f : \mathbb{R}^N \to \mathbb{R}$

$$y = f(\boldsymbol{x}) \,, \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$$

- Partial derivative (change one coordinate at a time):

$$\frac{\partial f}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_N) - f(\boldsymbol{x})}{h}$$

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- Jacobian vector (gradient) collects all partial derivatives:

$$\frac{df}{d\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{x_N} \end{bmatrix} \in \mathbb{R}^{1 \times N}$$

Note: This is a row vector.

Example

$$f : \mathbb{R}^2 \to \mathbb{R}$$
$$f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$$

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$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 x_2 + x_2^3$$
$$\frac{\partial f(x_1, x_2)}{\partial x_2} = x_1^2 + 3x_1 x_2^2$$

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- Gradient:

$$\frac{df}{d\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f(x_1,x_2)}{\partial x_1} & \frac{\partial f(x_1,x_2)}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 x_2 + x_2^3 & x_1^2 + 3x_1 x_2^2 \end{bmatrix} \in \mathbb{R}^{1\times 2}.$$

Rules

- Sum Rule

$$\frac{\partial}{\partial \boldsymbol{x}}\big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) = \frac{\partial f}{\partial \boldsymbol{x}} + \frac{\partial g}{\partial \boldsymbol{x}}$$

- Product Rule

$$\frac{\partial}{\partial \boldsymbol{x}}\big(f(\boldsymbol{x})g(\boldsymbol{x})\big) = \frac{\partial f}{\partial \boldsymbol{x}}g(\boldsymbol{x}) + f(\boldsymbol{x})\frac{\partial g}{\partial \boldsymbol{x}}$$

- Chain Rule

$$\frac{\partial}{\partial \boldsymbol{x}}(g \circ f)(\boldsymbol{x}) = \frac{\partial}{\partial \boldsymbol{x}}\big(g(f(\boldsymbol{x}))\big) = \frac{\partial g}{\partial f}\frac{\partial f}{\partial \boldsymbol{x}}$$

Example: Chain Rule

- Consider the function

$$L(\boldsymbol{e}) = \tfrac{1}{2}\|\boldsymbol{e}\|^2 = \tfrac{1}{2}\boldsymbol{e}^\top \boldsymbol{e}$$

$$\boldsymbol{e} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\,, \quad \boldsymbol{x} \in \mathbb{R}^N\,, \boldsymbol{A} \in \mathbb{R}^{M\times N}\,, \boldsymbol{e}, \boldsymbol{y} \in \mathbb{R}^M$$

- Compute $dL/d\boldsymbol{x}$. What is the dimension/size of $dL/d\boldsymbol{x}$?

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- Compute $dL/d\boldsymbol{x}$. What is the dimension/size of $dL/d\boldsymbol{x}$?
- $dL/d\boldsymbol{x} \in \mathbb{R}^{1\times N}$

$$\frac{dL}{d\boldsymbol{x}} = \frac{dL}{d\boldsymbol{e}}\frac{d\boldsymbol{e}}{d\boldsymbol{x}}$$

$$\frac{dL}{d\boldsymbol{e}} = \boldsymbol{e}^\top \in \mathbb{R}^{1\times M} \tag{1}$$

$$\frac{d\boldsymbol{e}}{d\boldsymbol{x}} = -\boldsymbol{A} \in \mathbb{R}^{M\times N} \tag{2}$$

$$\Rightarrow \frac{dL}{d\boldsymbol{x}} = \boldsymbol{e}^\top(-\boldsymbol{A}) = -(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})^\top \boldsymbol{A} \in \mathbb{R}^{1\times N}$$

$f : \mathbb{R}^N \to \mathbb{R}^M$

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^M, \quad \boldsymbol{x} \in \mathbb{R}^N$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} f_1(x_1, \ldots, x_N) \\ \vdots \\ f_M(x_1, \ldots, x_N) \end{bmatrix}$$

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- Jacobian matrix (collection of all partial derivatives)

$$\begin{bmatrix} \frac{dy_1}{d\boldsymbol{x}} \\ \vdots \\ \frac{dy_M}{d\boldsymbol{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{M \times N}$$

Example

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}\,, \qquad \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^M, \quad \boldsymbol{A} \in \mathbb{R}^{M\times N}, \quad \boldsymbol{x} \in \mathbb{R}^N$$

- Compute the gradient $d\boldsymbol{f}/d\boldsymbol{x}$
  - Dimension of $d\boldsymbol{f}/d\boldsymbol{x}$:

Example

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  - Gradient:

$$f_i = \sum_{j=1}^{N} A_{ij}x_j \qquad \Rightarrow \frac{\partial f_i}{\partial x_j} = A_{ij} \tag{3}$$

Example

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  - Gradient:

$$f_i = \sum_{j=1}^{N} A_{ij}x_j \qquad \Rightarrow \frac{\partial f_i}{\partial x_j} = A_{ij}$$

$$\Rightarrow \frac{d\boldsymbol{f}}{d\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} = \boldsymbol{A} \tag{3}$$

Chain Rule

$$\frac{\partial}{\partial \boldsymbol{x}}(g \circ f)(\boldsymbol{x}) = \frac{\partial}{\partial \boldsymbol{x}}\big(g(f(\boldsymbol{x}))\big) = \frac{\partial g}{\partial f}\frac{\partial f}{\partial \boldsymbol{x}}$$

Example

- Consider $f : \mathbb{R}^2 \to \mathbb{R}, \quad \boldsymbol{x} : \mathbb{R} \to \mathbb{R}^2$

$$f(\boldsymbol{x}) = f(x_1, x_2) = x_1^2 + 2x_2\,,$$

$$\boldsymbol{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \sin(t) \\ \cos(t) \end{bmatrix}$$

Example

- Consider $f : \mathbb{R}^2 \to \mathbb{R}, \quad \boldsymbol{x} : \mathbb{R} \to \mathbb{R}^2$

$$f(\boldsymbol{x}) = f(x_1, x_2) = x_1^2 + 2x_2\,,$$

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$$\frac{df}{dt} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix}$$

$$= \begin{bmatrix} 2 \sin t & 2 \end{bmatrix} \begin{bmatrix} \cos t \\ -\sin t \end{bmatrix}$$

$$= 2 \sin t \cos t - 2 \sin t = 2 \sin t (\cos t - 1)$$

BREAK

Derivatives with Matrices

- Re-cap: Gradient of a function $f : \mathbb{R}^D \to \mathbb{R}^E$ is an $E \times D$-matrix:

  # target dimensions × # parameters

  with

$$\frac{d\boldsymbol{f}}{d\boldsymbol{x}} \in \mathbb{R}^{E \times D}, \qquad df[e,d] = \frac{\partial f_e}{\partial x_d}$$

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- Generalization to cases, where the parameters (D) or targets (E) are matrices, apply immediately
- Assume $f : \mathbb{R}^{M\times N} \to \mathbb{R}^{P\times Q}$, then the gradient is a $(P \times Q) \times (M \times N)$ object (tensor) where

$$df[p,q,m,n] = \frac{\partial f_{pq}}{\partial X_{mn}}$$

Derivatives with Matrices: Example (1)

$$\boldsymbol{f} = \boldsymbol{A}\boldsymbol{x}\,, \quad \boldsymbol{f} \in \mathbb{R}^M, \boldsymbol{A} \in \mathbb{R}^{M\times N}, \boldsymbol{x} \in \mathbb{R}^N$$

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$$\frac{d\boldsymbol{f}}{d\boldsymbol{A}} \in \mathbb{R}^{M\times(M\times N)}$$

$$\frac{d\boldsymbol{f}}{d\boldsymbol{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \boldsymbol{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \boldsymbol{A}} \end{bmatrix}, \quad \frac{\partial f_i}{\partial \boldsymbol{A}} \in \mathbb{R}^{1\times(M\times N)}$$

Derivatives with Matrices: Example (2)

$$f_i = \sum_{j=1}^{N} A_{ij} x_j, \quad i = 1, \ldots, M \tag{4}$$

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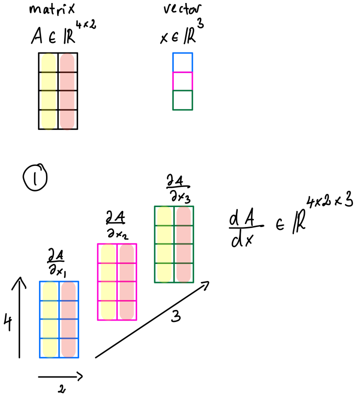
$$\frac{\partial f_i}{\partial \boldsymbol{A}} = \begin{bmatrix} \mathbf{0}^\top \\ \vdots \\ \boldsymbol{x}^\top \\ \mathbf{0}^\top \\ \vdots \\ \mathbf{0}^\top \end{bmatrix} \in \mathbb{R}^{1\times(M\times N)} \tag{4}$$

Example: Higher-Order Tensors

- Consider a matrix $\boldsymbol{A} \in \mathbb{R}^{4\times 2}$ whose entries depend on a vector $\boldsymbol{x} \in \mathbb{R}^3$
- We can compute $d\boldsymbol{A}(\boldsymbol{x})/d\boldsymbol{x} \in \mathbb{R}^{4\times 2\times 3}$ in two equivalent ways:



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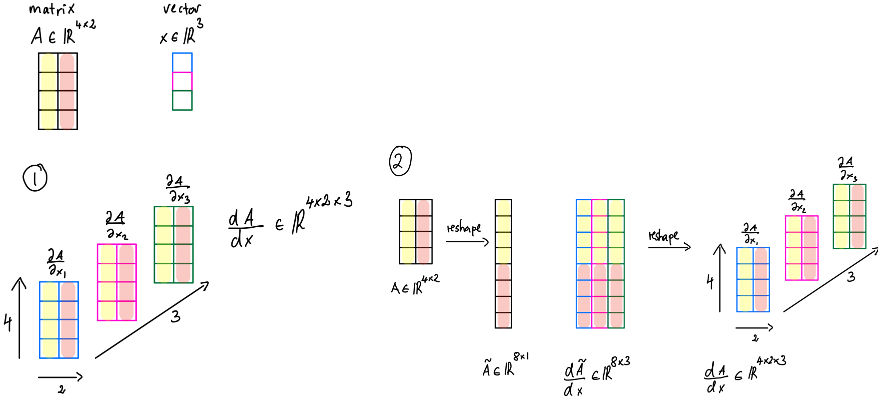
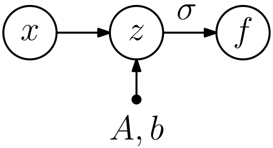


Gradients of a Single-Layer Neural Network (1)



$$\boldsymbol{f} = \tanh(\underbrace{\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}}_{=:\boldsymbol{z}\in\mathbb{R}^M}) \in \mathbb{R}^M, \quad \boldsymbol{x} \in \mathbb{R}^N, \boldsymbol{A} \in \mathbb{R}^{M\times N}, \boldsymbol{b} \in \mathbb{R}^M$$

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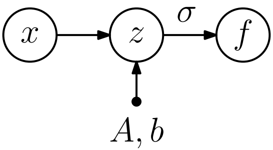

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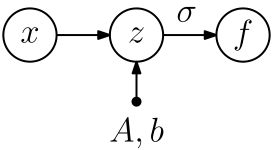

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```
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```

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$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{A}}$$ ▶▶ See (4)

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```
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Putting Things Together

- Inputs $\boldsymbol{x}$, observed outputs $\boldsymbol{y} = f(\boldsymbol{z}, \boldsymbol{\theta}) + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma})$

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- Find $\boldsymbol{A}, \boldsymbol{b}$, such that the squared loss

$$L(\boldsymbol{\theta}) = \tfrac{1}{2}\|\boldsymbol{e}\|^2\,, \quad \boldsymbol{e} = \boldsymbol{y} - \boldsymbol{f}(\boldsymbol{z}, \boldsymbol{\theta})$$

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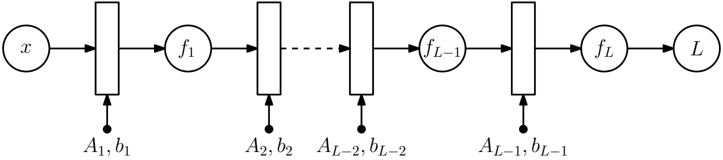
- Partial derivatives:

$$\left.\begin{aligned} \frac{\partial L}{\partial \boldsymbol{A}} &= \frac{\partial L}{\partial \boldsymbol{e}} \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{A}} \\ \frac{\partial L}{\partial \boldsymbol{b}} &= \frac{\partial L}{\partial \boldsymbol{e}} \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}} \end{aligned}\right\} \quad \frac{\partial L}{\partial \boldsymbol{e}} \blacktriangleright\blacktriangleright (1) \quad \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} \blacktriangleright\blacktriangleright (2), (3) \quad \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} \blacktriangleright\blacktriangleright (6) \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{A}} \blacktriangleright\blacktriangleright (4) \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}} \blacktriangleright\blacktriangleright (5)$$

Gradients of a Multi-Layer Neural Network



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$$\boldsymbol{f}_0 = \boldsymbol{x}$$

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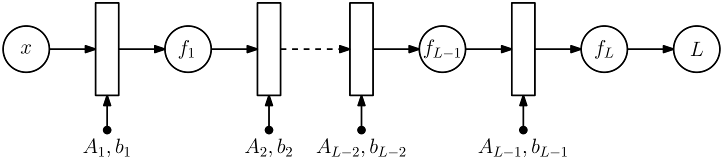

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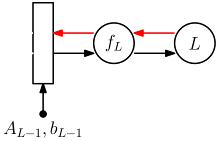
- Find $\boldsymbol{A}_j, \boldsymbol{b}_j$ for $j = 0, \ldots, L-1$, such that the squared loss

$$L(\boldsymbol{\theta}) = \|\boldsymbol{y} - \boldsymbol{f}_L(\boldsymbol{\theta}, \boldsymbol{x})\|^2$$

is minimized, where $\boldsymbol{\theta} = \{\boldsymbol{A}_j, \boldsymbol{b}_j\}, \quad j = 0, \ldots, L-1$

Gradients of a Multi-Layer Neural Network



$$\frac{\partial L}{\partial \boldsymbol{\theta}_{L-1}} = \frac{\partial L}{\partial \boldsymbol{f}_L} \frac{\partial \boldsymbol{f}_L}{\partial \boldsymbol{\theta}_{L-1}}$$

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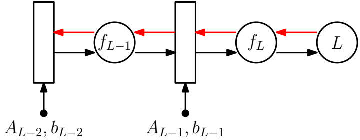

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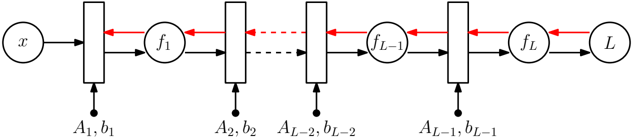

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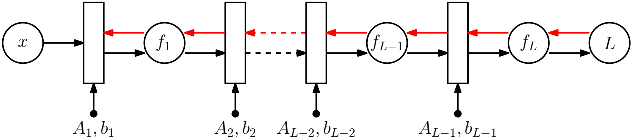
Gradients of a Multi-Layer Neural Network



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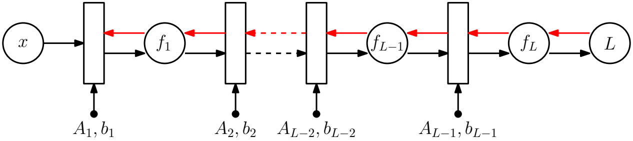
Gradients of a Multi-Layer Neural Network



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▸▸ More details (including efficient implementation) later this week

Training Neural Networks as Maximum Likelihood Estimation

- Training a neural network in the above way corresponds to maximum likelihood estimation:
  - If $\boldsymbol{y} = NN(\boldsymbol{x}, \boldsymbol{\theta}) + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$ then the log-likelihood is

$$\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) = -\tfrac{1}{2}\|\boldsymbol{y} - NN(\boldsymbol{x}, \boldsymbol{\theta})\|^2$$

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- Maximum likelihood estimation can lead to overfitting (interpret noise as signal)

Example: Linear Regression (1)

- Linear regression with a polynomial of order M:

$$y = f(x, \boldsymbol{\theta}) + \epsilon\,, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_\epsilon^2\big)$$

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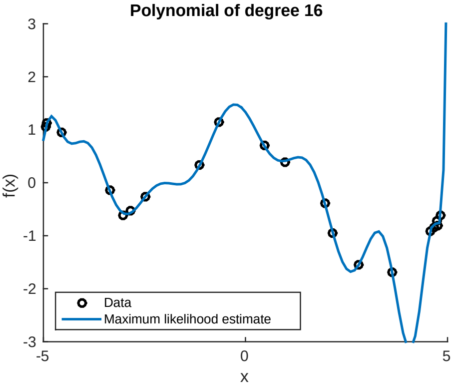
- Given inputs x_i and corresponding (noisy) observations y_i, $i = 1, \ldots, N$, find parameters $\boldsymbol{\theta} = [\theta_0, \ldots, \theta_M]^\top$, that minimize the squared loss (equivalently: maximize the likelihood)

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{N} (y_i - f(x_i, \boldsymbol{\theta}))^2$$

Example: Linear Regression (2)



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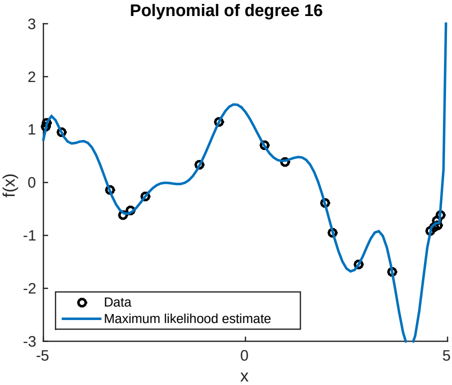


- Regularization, model selection etc. can address overfitting
  ▶▶ Tutorials later this week
- Alternative approach based on integration

Overview

Introduction

Differentiation

Integration

Integration: Outline

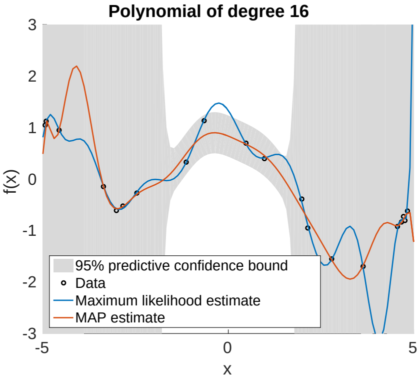
1. Motivation
2. Monte-Carlo estimation
3. Basic sampling algorithms

Bayesian Integration to Avoid Overfitting

- Instead of fitting a single set of parameters $\boldsymbol{\theta}^*$, we can average over all plausible parameters

  ▶▶ Bayesian integration:

$$p(\boldsymbol{y}|\boldsymbol{x}) = \int p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$$



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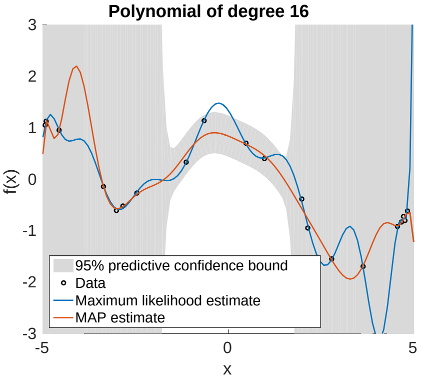

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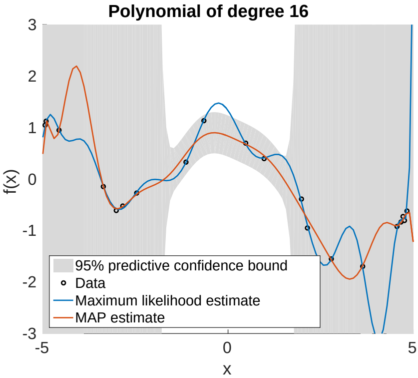

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- For neural networks this integration is intractable
  ⏩ Approximations

Computing Statistics of Random Variables

- Computing means/(co)variances also requires solving integrals:

$$\mathbb{E}_x[\boldsymbol{x}] = \int \boldsymbol{x} p(\boldsymbol{x}) d\boldsymbol{x} =: \boldsymbol{\mu}_x$$

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- These integrals can often not be computed in closed form

▸▸ Approximations

Approximate Integration

- Numerical integration (low-dimensional problems)
- Bayesian quadrature, e.g., O'Hagan (1987, 1991); Rasmussen & Ghahramani (2003)
- Variational Bayes, e.g., Jordan et al. (1999)
- Expectation Propagation, Opper & Winther (2001); Minka (2001)
- **Monte-Carlo Methods**, e.g., Gilks et al. (1996), Robert & Casella (2004), Bishop (2006)

Monte Carlo Methods—Motivation

- Monte Carlo methods are computational techniques that make use of random numbers
- Two typical problems:
  1. **Problem 1:** Generate samples $\{\boldsymbol{x}^{(s)}\}$ from a given probability distribution $p(\boldsymbol{x})$, e.g., for simulation or representations of data distributions

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▶▶ Example: Means/variances of distributions, predictions

Complication: Integral cannot be evaluated analytically

Problem 2: Monte Carlo Estimation

- Computing expectations via statistical sampling:

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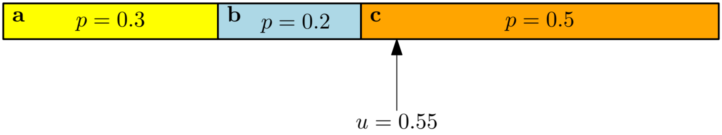
- **Key problem:** Generating samples from $p(\boldsymbol{x})$ or $p(\boldsymbol{\theta})$

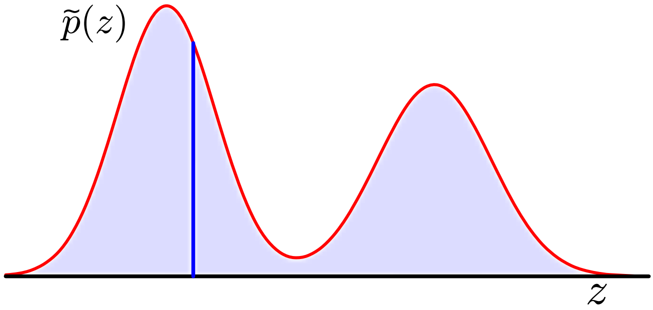
  ▶▶ Need to solve **Problem 1**

Sampling Discrete Values



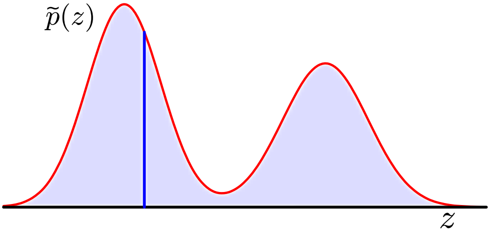
- $u \sim \mathcal{U}[0, 1]$, where $\mathcal{U}$ is the uniform distribution
- $u = 0.55 \Rightarrow x = c$

Continuous Variables



- More complicated
- Geometrically, we wish to sample uniformly from the area under the curve
- Two algorithms here:
  - Rejection sampling
  - Importance sampling

Rejection Sampling: Setting



- Assume:
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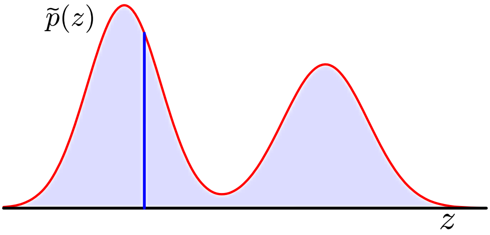
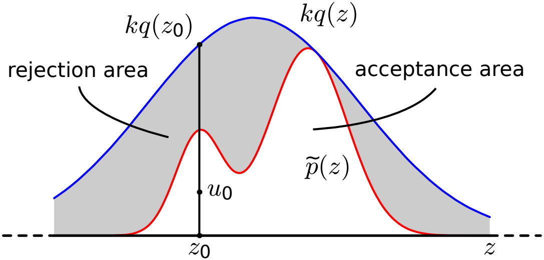


- Assume:
  - Sampling from $p(z)$ is difficult
  - Evaluating $\tilde{p}(z) = Zp(z)$ is easy (and Z may be unknown)
- Find a simpler distribution (proposal distribution) $q(z)$ from which we can easily draw samples (e.g., Gaussian, Laplace)
- Find an upper bound $kq(z) \geqslant \tilde{p}(z)$

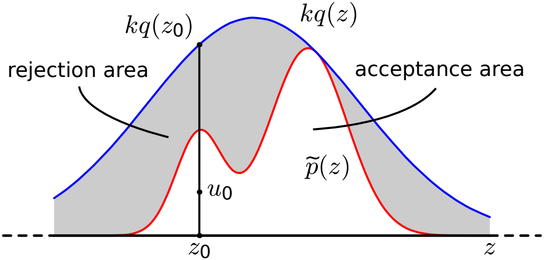
Rejection Sampling: Algorithm



Adapted from PRML (Bishop, 2006)

1. Generate $z_0 \sim q(z)$
2. Generate $u_0 \sim \mathcal{U}[0, kq(z_0)]$
3. If $u_0 > \tilde{p}(z_0)$, reject the sample. Otherwise, retain z_0

Properties



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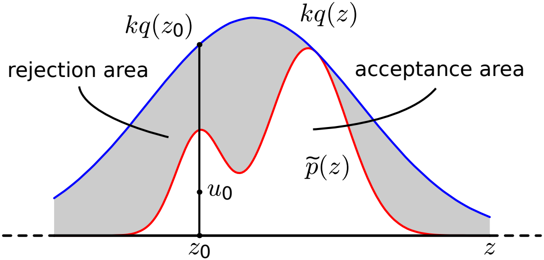

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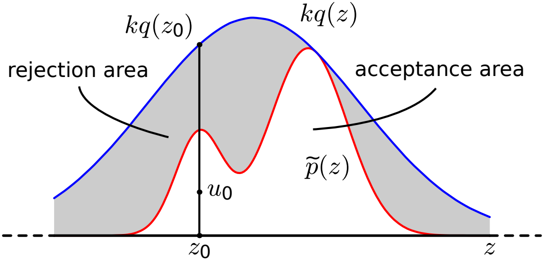

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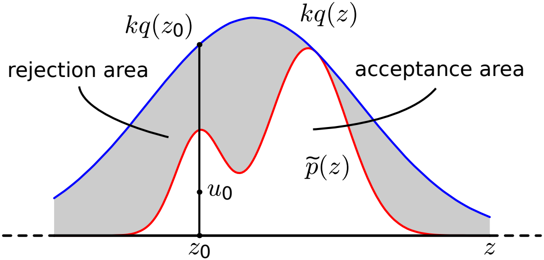
- Probability density of the z-coordiantes of accepted points must be proportional to $p(z)$
- Samples are independent samples from $p(z)$

Shortcomings



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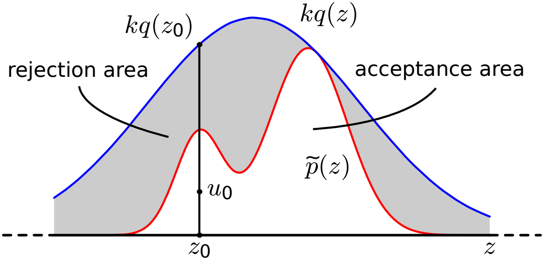

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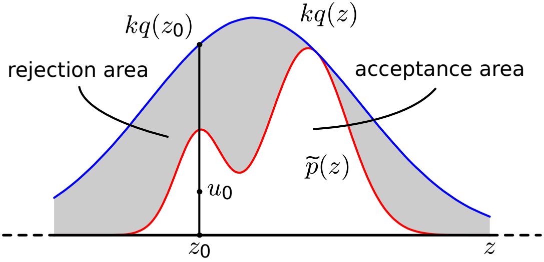

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- Finding the upper bound k is tricky
- In high dimensions the factor k is probably huge
- **Low acceptance rate/high rejection rate** of samples

Importance Sampling

Key idea: Do not throw away all rejected samples, but give them lower weight by rewriting the integral as an expectation under a simpler distribution q (proposal distribution):

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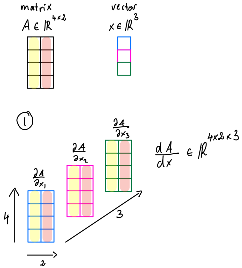
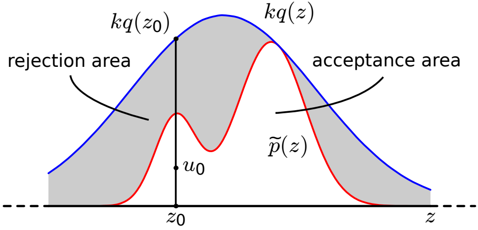
▸▸ Different approach to sample from complicated (high-dimensional) distributions: Markov Chain Monte Carlo (e.g., Gilks et al., 1996)

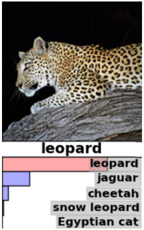
Summary

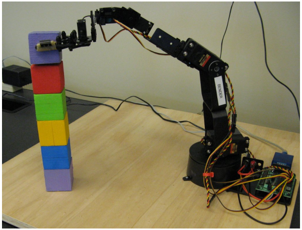


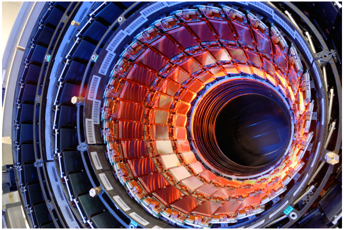


- Two mathematical challenges in machine learning
  - **Differentiation** for optimizing parameters of machine learning models
    ⏩ Vector calculus and chain rule
  - **Integration** for computing statistics (e.g., means, variances) and as a principled way to address overfitting issue
    ⏩ Monte-Carlo integration to solve intractable integrals

Some Application Areas







- Image/speech/text/language processing using deep neural networks (e.g., Krizhevsky et al., 2012 or overview in Goodfellow et al., 2016)
- Data-efficient reinforcement learning and robot learning using Gaussian processes (e.g., Deisenroth & Rasmussen, 2011)
- High-energy physics using deep neural networks or Gaussian processes (e.g., Sadowski et al. 2014; Bertone et al., 2016)

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