Advanced Machine Learning

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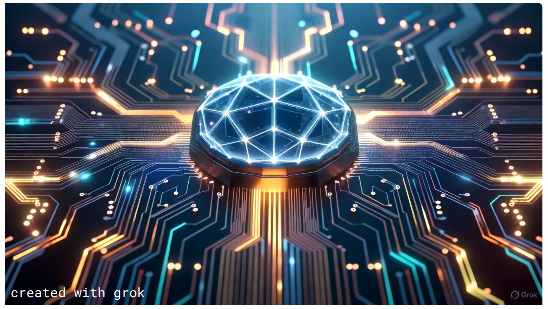
github.com/silvasta/summary-aml



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Representation

1 Learning objectives

Estimation of Dependences Based on Empirical Data

What is the learning problem?

$$y = f_\theta(x) + \eta \quad \text{with} \quad \nu \sim \mathsf{P}(\eta|0, \sigma^2)$$

2 Expected risk

- Conditional expected risk

- Total expected risk

3 Empirical risk

- Test and Train Data

Test data cannot be used before the final estimator has been selected!

Training error $\hat{R}\hat{(}f_n, \mathcal{Z}^{\text{train}})$ for Empirical Risk Minimizer (ERM) $\hat{f}_n$

4 Empirical test error and expected risk

Distinguish

5 Comparing algorithm performance on test data

6 Data

6.1 Feature space

- Measurement space $\mathcal{X}$

+ numerical $\mathcal{X} \subset \mathbb{R}^d$

+ boolean $\mathcal{X} = \mathbb{B}$

+ categorial $\mathcal{X} = \{1, ..., k\}$

Features are derived quantities or indirect observations which often significantly compress the information content of measurements.

Remark The selection of a specific feature space predetermines the metric to compare data; this choice is the first significant design decision in a machine learning system.

Taxonomy of Data

6.2 Example of Data

- monadic data

- dyadic data

- pairwise data

- polyadic data

7 Mathematical Spaces

- Topological spaces

- Metric space

- Euclidean vector spaces

- Probability Spaces

Regression

8 Linear Regression

- Statistical model

$$Y = X^\top \beta. \quad Y \in \mathbb{R}. \, X.\beta \in \mathbb{R}^{d+1}$$

- Residual Sum of Squares (RSS)

$$RSS(\beta) \; = \; (\mathbf{y} - \mathbf{X}\beta)^\top (\mathbf{y} - \mathbf{X}\beta)$$
$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

9 Gauss Markov Theorem

10 Bias/Variance Dilemma

- Tradeoff, split Error

- Identify error components

11 Bayesian Maximum A Posteriori (MAP) estimates

11.1 Ridge Regression

- Cost function

- Bayesian view

- Solution

Tikhonov regularization

11.2 LASSO

- Cost function

- Bayesian view

- Solution

11.3 Ridge vs. LASSO Estimation

12 Remarks on Shrinkage Methods

- Generalized Ridge Regression

Idea behind shrinkage When white noise is added to the data then all Fourier coefficients are increased by a constant on average. ▯ Shrink all coefficients by the estimated noise amount to derive a robust predictor.

13 Learning Objectives

- To motivate, understand, and design Gaussian processes.

- To be able to analytically derive procedures for making predictions with Gaussian processes.

- To analytically compute conditionals, marginals, and posteriors of Gaussians.

- To formulate and understand kernels.

- To be able to use kernel engineering to design new kernels.

- To be able to make a formal connection between Gaussian processes and Bayesian linear regression.

14 Gaussian Processes

14.1 Bayesian linear regression

multiple linear regression model

$$Y = X^T\beta + \epsilon \quad \text{Gaussian Noise } \epsilon \sim \mathcal{N}(\epsilon|0, \sigma^2)$$

$$p(Y|X, \beta, \sigma) = \mathcal{N}(Y|X^T\beta, \sigma^2) \propto e^{-\frac{1}{2\sigma^2}(Y-X^T\beta)^2}$$

Bayesian linear regression extends multiple linear regression by defining a prior over the regression coefficients, for example (ridge regression)

- Model inversion

14.2 Moments of Bayesian linear regression

Setting

Expected Value

Covariance

15 Gaussian processes

Moments of joint Gaussian:

$Y \sim \mathcal{N}(Y|0, k_{i,j} + \sigma^2 \text{if } i = j)$

with $k_{i,j}$ kernel function

Gaussian Processes as "kernelized linear regression"

- Kernel functions specify the similarity between any two data points.

15.1 Recall

Kernel properties:

- Symmetry

- Positive semi-definit

15.2 Gram matrix

Must be positive semi-definit

$$K = \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & & \vdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{bmatrix}$$

15.3 Examples of kernel functions

Linear kernel: k(x, x0) = xT x0

Polynomial kernel: k(x, x0) = (xT x0 + 1)p , for p ▯ N

Gaussian (RBF) kernel: k(x, x0) = exp −kx − x0 k22 /h2

Sigmoid (tanh) kernel: k(x, x0) = tanh κxT x0 − b

Different kernels have different **invariance properties**!

For example, invariance to **rotation** or **translation.**

15.4 Kernel engineering by composition

Addition: Multiplication: Scaling: Composition:

15.5 Prediction by Gaussian processes

Predictive density $p(y_{n+1}|x_{n+1}, X, y)$

Reminder: Conditional Gaussian Distributions

15.6 Prediction by Gaussian processes

15.7 Kernel validation

Goal: Validate hyperparameters of kernels by random splits D

16 Controller Optimization for Robust Control

Machine Learning in Control Systems

Machine learning techniques are becoming more and more important for enabling computers to control complex and stochastic systems and predict the outcomes of such systems.

16.1 Gaussian processes for Control

A Fundamental problem when designing controllers for dynamic systems is the estimation of the controller parameters. Besides pure statistical performance, robustness arises as an important design issue.

The classical approach selects a model of the system to design an initial controller; parameters are then tuned manually to achieve best performance.

An alternative approach uses methods from machine learning to optimize statistical performance, e.g., Bayesian optimization.

Safety-critical system failures may happen because these methods evaluate different controller parameters.

16.2 Safe optimization

Overcome safety-critical system failures by using a specialized optimization algorithm for automatic controller parameter tuning. This algorithm models the underlying performance measure as a GP and only explores new controller parameters whose performance lies above a safe performance threshold with high probability.

17 Model averaging is common practice

- Previous: Gaussian process motivated by Bayesian linear regression.

- Seldom: take MAP estimator in Bayesian setting.

- Bayesian approach: average models with different parameters (weighted according to prior).

- Cross validation: Take average over models trained on different folds.

- Winners of most Machine Learning competitions (e.g. on Kaggle): ensembles (weighted averages of models).

-

18 Combining Regressors - Bias

TODO: formula

-

19 Combining Regressors - Variance

TODO: formula

20 Ensemble Learning

The idea of classifier ensembles Boosting is an approach to machine learning based on the idea of creating a highly accurate prediction rule by combining many relatively weak and inaccurate rules.

- Computational advantage

- Statistical advantage

21 Induction Principles for Classifier Selection

I) Empirical Risk Minimization (ERM) Principle

II) Bayesian inference by model averaging

22 Motivation for Ensemble Methods

- Train several sufficiently diverse predictors

- Bagging

- Arcing

- Boosting

23 Weak Learners Used for Bagging or Boosting

Combining Classifiers

Bagging Classifiers

Classifier selection: First compare, then bag!

Bagging: The Mechanism

Decision Trees

Random Forests

The Idea of Boosting

AdaBoost

Data Reweighting

Boosted Classifier

Comparison of ensemble methods

24 Loss functions for classification

Support Vector Machines

25 SVM and convex optimization

25.1 Learning objectives

- Lagrange multipliers

- Basics of convex optimization and duality

25.2 Instability of the perceptron

25.3 Maximum-margin criterion

25.4 Lagrange Multipliers

25.5 Convex optimization

The dual

Weak duality and strong duality

Slater's condition

Consequences of strong duality

− The primal optimal solution is the minimizer of the Lagrangian:

− Complementary slackness:

Convex optimization via the dual

25.6 SVMs

- Formula seperation band

- Projection

- Normalization trick

- Formalizatin of primal

Why do we compute the dual?

- SVM calculation can become intractable in high dimensions or when working with transformations (more on this later).

- The dual does not depend on the dimensionality of the dataset in the primal!

Complementary slackness

What about the intercept?

What if the dataset is not linearly separable?

- Soft-margin SVMs

- Kernels

25.7 Soft-margin SVMs

- Formulation

- The role of C

dual ...

26 Kernelization

Transformations and kernels

Polynomial transformations

SVMs and kernels

26.1 Kernels

no need for ϕ only $\phi^T(x)\phi(x')$ for some cases of x and x'

27 SVM summary

Support Vector Machine (SVM): Idea

- margin

- kernel

Nonlinear Transformation in Kernel Space

SVM Lagrangian for functional margin formulation

Non-separable case: Soft Margin SVM

Learning the Soft Margin SVM

28 Structural SVMs

From margins to score functions

Extensions to the SVM

Multiclass SVMs (linear discriminant function)

Structural SVMs

..more examples

Neural Networks

- Activation functions

- Forward computation

- Gradient descent

- Chain rule

A **computation DAG** is a directed acyclic graph where vertices are annotated with variables and edges are annotated with differentiable vector fields.

- generalization chain rule

- Backward computation

Transformer

29 Tokenization and embeddings

- Topic classification

Strategy for NLP

We create for each word in the sentence an embedding vector. Then we aggregate these embeddings to create an embedding for the sentence. We then apply a function on the embedding to map the sentence to a distribution of topics.

- Tokenization

The first step is to transform the sentence into a sequence of tokens.

A popular method is the WordPiece tokenization. It produces a decomposition of a training corpus of text into S tokens, where S is predefined in advance.

1. Set T = set of characters occurring in text

2. While size of T > S do:

1. Find the most common pair a, b of tokens in T occurring in the text.

2. Remove a and b from T and put instead a new token ab in T.

30 Self-attention

- Sentiment classification for movies

- Attention

- Relational matrices

These maps can also be used to infer meanings from words

Every word finds its meaning through other words in the sentence!

Attention as information retrieval

An attention map for location of objects

- Query

- Keys

- Values

Abstraction of an attention mechanism

30.1 Multi-headed attention

30.2 Cross-attention

Consider the problem of translating from English to German:

- A different attention mechanism is needed

Abstraction of a cross-attention mechanism

30.3 Masked self-attention

Consider the task of generating text for answering questions.

31 Positional encodings

- Consider the sentences the dog chased the cat and the cat chased the dog.

- They are permutations of each other, so the attention maps will also just be permutations of each other.

- Note that attention mechanisms do not pay attention to the position of a token in the sentence.

- Binary positional encoding

- Positional encodings

Why adding and not contatenating?

32 Broadcasting

- Broadcasting in PyTorch

- Examples of broadcasting

Broadcasting formalized

Implementing the masked-attention mechanism

33 Residual Blocks

- The degradation problem

- Residual blocks

34 Transformer Architecture

BERT: Bidirectional Encoder Representations from Transformers

Computer Vision

35 CNNs and UNets

35.1 Convolutions and deconvolutions

Convolutional filters

- Input feature map (5x5)

- Padding (2)

- Kernel size (3x3)

- Stride (4)

Deconvolutional filters

Convolutional and deconvolutional layers

- A (de)convolutional layer consists of a number of equally-sized (de)convolutional filters, a padding, and a stride.

- The output is a tensor where the number of channels matches the number of filters in the layer.

35.2 U-net

- A typical architecture for image segmentation.

- One can also treat a U-net as some sort of image autoencoder

- Image from original paper: https://arxiv.org/abs/1505.04597

36 Stable diffusion

36.1 Diffusion models with images

Denoising diffusion probabilistic models (DDPM) (Ho et al, 2020)

Forward process

Reverse process

36.2 Conditional diffusion processes

37 Neural networks and variational autoencoder

37.1 Clip

Autoencoders create their own representations

This prevents the decoding as text of image representations produced by an encoder.

How can we harmonize such representations?

38 Stable diffusion

Goal

Given a text prompt, produce an image associated to that prompt.

Idea

Produce text and image embeddings that are semantically relatable.

When given a text, we produce an embedding and then use a generative model to produce an image, guided with the text.

38.1 Semantically relatable text embeddings with CLIP

1. Select an image and a text encoder.

2. Encode all images and texts.

3. Transform all embeddings to the same Euclidean space.

4. Compute a similarity matrix containing all similarities between each pair of text-image embeddings.

5. Maximize the diagonal elements and minimize the non-diagonal elements.

38.2 Cross-attention

We need a cross-attention mechanism for images and texts.

Multi-headed cross-attention mechanism for UNets

39 ViTs and MAEs

39.1 Vision transformers

39.2 Masked auto encoders

Image encoding vs text encoding

Images are signals with very heavy spatial redundancy. Words are signals with low redundancy.

Pixels have little semantic information. Words have high semantic information.

Principle for an image autoencoder

- Remove a large fraction of the image, and create the encoding from there. Then learn to reconstruct the image from only those encodings.

Diffusion

Lecture 8, 03.11.25

Diffusion (to produce images)

- goal find $p^\star$

- Start with gaussian distribution

- generative process, from noise to image

- corruptive process, from image sample to noise

Training

corruptive process

x(i) image

$e_t(i) \to x_t(i)$

up to the middle / noise

reverse process

from noise to image

Diffusion process for MNIST

39.3 sgrok

Diffusion Models for Image Generation

Diffusion models are a class of generative models aimed at producing images by learning to approximate the true data distribution $p^\star$. The core idea involves two complementary processes: a **corruptive process** that gradually adds noise to an image, transforming it into pure Gaussian noise, and a **reverse process** that denoises the noise back to a realistic image.

Corruptive Process (Forward Diffusion) Starting from a clean image sample $x_0(i)$ (e.g., a digit from the MNIST dataset), the corruptive process applies a sequence of noise additions over T timesteps:

$$x_t(i) = \sqrt{\alpha_t} x_{t-1}(i) + \sqrt{1-\alpha_t}\epsilon_t(i), \quad \epsilon_t(i) \sim \mathcal{N}(0, I),$$

where α_t controls the noise level, and $\epsilon_t(i)$ is Gaussian noise. This continues until $x_T(i)$ approximates a standard Gaussian distribution (pure noise) at timestep T, effectively destroying the image structure.

Training During training, the model learns to reverse this corruption. A neural network (e.g., a U-Net) is trained to predict the noise $\epsilon_t(i)$ added at each timestep t, given the noisy image $x_t(i)$. The objective is to minimize the difference between predicted and actual noise, often using a mean-squared error loss. This allows the model to capture the data distribution by simulating the forward process on training samples (like MNIST digits) and optimizing the reverse denoising steps.

Generative Process (Reverse Diffusion) For generation, start with a sample from a Gaussian distribution (pure noise) $x_T \sim \mathcal{N}(0, I)$. The trained model iteratively denoises it via the reverse process:

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \hat{\epsilon}_t(x_t) \right) + \sigma_t z, \quad z \sim \mathcal{N}(0, I$$

where $\hat{\epsilon}_t$ is the model's noise prediction, and $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$. Over T steps, this transforms noise into a high-fidelity image, such as a synthetic MNIST digit.

This framework, as in Denoising Diffusion Probabilistic Models (DDPM), excels in tasks like image synthesis due to its stable training and high-quality outputs. For implementation, engineers can use libraries like Diffusers (Hugging Face) with pre-trained models for MNIST or extend to advanced variants like Stable Diffusion for conditional generation.

39.4 Encoder

Autoencoder

Clip

- encode image and text

- match them somehow

- produce like diagonal matrix

39.5 Pipeline

Goal: text to image

Idea:

- produce text and image embeddings that are semantically relatable

- text -> produce embedding -> generative model -> image

details

- cross attention

39.6 Unet Architecture

prompt -> encoder -> embeding-text

image -> encoder ->et -> corrupted image xt

xt -> unet (only image input), now?

add text with cross-attention inbetween UNet steps

Multi-headed X Attention Mechanism

embeding-text (Batch,MaxTokens,DimEmbeddings)

embeding-image (Batch,Chanels, Heigth, Width)

wK,wV to Et, gives K(B,F,M,Dk),V(B,F,M,Dv)

wQ to Ei, gives Q

- calculate similarities

use K,Q to create P(B,F,M,H,W)

- P = similarity of token m in text and pixel (h,w) of image

create S, softmax of P (along dimension M)

Create A(B,F,Dv,H,W) from S and V

use wO(Do,H,W) to create output Ao(B,Do,H,W)

Graph Neural Networks

40 Graph

Toxic, non toxic? structure matters -> graph

G(V,E)

V=1,...,N

$Ec = V \times V$

Anomaly Detection

Reinforcement Learning

Exercises

41 Problem 1 - Regression

- Linear Regression

- Ridge Regression

- Noisy Regression

E1.2.c - An Engineer's rule of thumb is to choose K as min $\sqrt{n}, 10$

- Overfitting

- Cross Validation

- Generative vs. Discriminative Modeling