Machine Learning Concepts

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November 9, 2023

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1 Convexity

• If f is a differentiable convex function and $\nabla f(w) = 0$, then w is the global minimum of f.

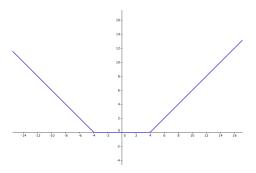


Figure 1: Convex function illustration

- Even if it is not strongly convex, it has a global minimum, just not only
 one.
- Attention: Just being differentiable and convex doesn't mean it has a stationary point: $f(w^{t+1}) < f(w^t)$.

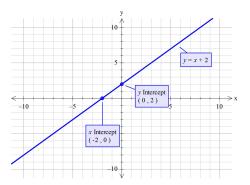


Figure 2: Convex but has no maximum, minimum, saddle point

• Only a strong convex function implies a semi-definite positive Hessian matrix.

2 Gradient Descent

Consider the gradient descent algorithm for minimizing a differentiable function f with iterates $w^{t+1} = w^t - \eta \nabla f(w^t)$. Suppose that $||\nabla f(w^t)|| > 0$. Then there always exists a step-size $\eta > 0$ such that.

Attention: This is only the case for gradient descent and not stochastic gradient descent!

3 Discriminative vs Generative Models

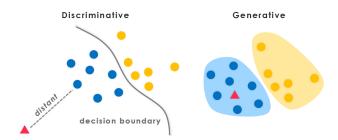


Figure 3: Difference between discriminative and generative models

Description	Discriminative	Generative
What is modeled	P(y x)	P(x,y)
What is learned	Decision boundary	Probability distribution of data
Example	SVM, logistic regression	Gaussian Bayes classifier, GANS
Advantage	Cheaper, less prone to overfitting	Good at detecting outliers, generate new data

4 Gaussian Bayes Classifier (GBC)

How is P(x, y) modeled?

$$\begin{split} P(x,y) &= P(y) \cdot P(x|y) \\ P(Y=y) &= \text{Categorical Distribution} \\ P(X=x|Y=y) &= \text{XI}(x; M_y, \sum_y) \end{split}$$

5 Convolutional Neural Network (CNN)

A convolutional neural network consists of an input layer, hidden layers, and an output layer. In a CNN, the hidden layers include one or more layers that perform convolutions.

In a CNN, the input is a tensor with shape: (number of inputs) \times (input height) \times (input width) \times (input channels). After passing through a convolutional layer, the image becomes abstracted to a feature map, also called an activation map, with shape: (number of inputs) \times (feature map height) \times (feature map width) \times (feature map channels).

Parameters =
$$K \times K \times K \times C \times F$$

A higher threshold leads to fewer positive predictions, reducing the false positive rate for higher thresholds.

6 Ridge Regression

- Has increased bias for decreased variance.
- Closed form: $w^{\text{ridge}}(\lambda) = (X^T X + \lambda I^d)^{-1} X^T y$
- Has very low weighted values.
- Regularization tries to keep weights small.

7 Lasso Regression

- Has no closed-form solution.
- Has zero values.

8 Ordinary Least Squares

- Augmenting the set of features used for the regression will never increase the least squares loss.
- Subtracting the empirical mean from the data before performing regression on the centered samples.

9 Support Vector Machine (SVM)

- Support vectors are the closest to the boundary.
- Unconstrained soft-margin SVM is an l_2 -penalized hinge loss.

10 Expectation-Maximization (EM) Algorithm

- EM algorithm converges to a local maximum/saddle point, not only with careful initialization.
- Every iteration of the EM algorithm increases the marginal likelihood of the data.
- Instead of the EM algorithm, it is possible to adapt gradient descent for learning the parameters of the GMM and its latent assignments.

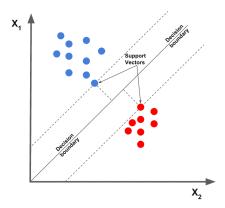


Figure 4: Support Vector Machine

- Doesn't have step size.
- Iterative optimization algorithm used to estimate the parameters of probabilistic models when some data is missing or unobserved.

11 Gaussian Mixture Model

- Probabilistic model used for representing complex data distributions.
- Works well when data is believed to be generated from a mixture of Gaussian distributions.
- Parameters of GMM:
 - Means: Represent the center of each component.
 - Covariance: Controls the shape and orientation of the component.
 - Mixing coefficients: Relative contribution of each component to the overall distribution.
- Trained using Expectation-Maximization (EM) algorithm.

12 Bootstrap

- 12.1 Advantage of using bootstrap parameter estimates in comparison with distribution-dependent parameter estimates
 - There is no closed-form solution for bootstrap parameter estimates.

- Bootstrap sampling is a way of artificially creating more datasets. Basically, you take random samples from the dataset with replacement.
- Sampling with replacements makes it
- computationally expensive.
- Bootstrapping is possible for any ML technique, as it can be computed for any black-box predictor.
- Bootstrap estimates are not asymptotically stable.

13 Generative Adversarial Networks

D: discriminator G: neural network generator

- If D and G both have enough capacity, i.e., if they can model arbitrary functions, the optimal G will be such that $G(z) \sim p_{data}$.
- The objective can be interpreted as a two-player game between G and D.
- The output of the discriminator is the probability of classifying x as being real:

$$1 - D_G(x)$$

14 Naive Bayes Classifiers

- Every pair of features being classified is independent of each other.
- Bayes' Theorem:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

15 Error

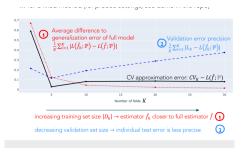


Figure 5: Error

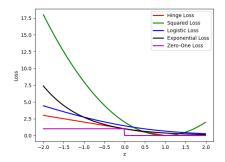


Figure 6: Error types

• Logistic: Minimum is at ∞ .

• Square:

- Well-defined minimum, but the point is that this minimum (at 1) seems a bit random and does not make a lot of sense.

• Exponential:

- Penalizes wrong labels very much and very quickly. Even one error could heavily penalize your model.
- Has exploding derivatives for wrong results and therefore is unstable.

• Hinge:

- For SVM.
- Is convex.
- Has a minimum.
- Not differentiable at 1.

• Logistic:

- For cross-entropy.
- Differentiable at all points.
- Models conditional probability p(y|w,x).
- The logistic loss doesn't necessarily maximize the margin between classes since it takes into account all the samples in both classes.

• Linear:

 Too sensitive to outliers and returns garbage when there is an imbalance in data.

• 0-1-Loss:

- Derivative is always 0, doesn't make sense to optimize that.

• Cross-Entropy Loss in Classification:

- Cross-entropy loss is a crucial component in training classification models.
- It quantifies the dissimilarity between predicted class probabilities and actual class labels.
- For each data point, the cross-entropy loss is computed by taking the negative logarithm of the predicted probability assigned to the true class:

$$L_i = -\sum_{k=1}^K y_{ik} \cdot \log(p_{ik})$$

- This loss function not only measures the correctness of the model's predictions but also encourages the model to be confident and accurate in its class probability assignments.
- The overall objective during training is to minimize the mean cross-entropy loss across the dataset:

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i$$

16 Asymmetric 0-1 Loss with Abstention

We shall define a new loss named 0-1 loss with abstention with an *extended* action space:

$$f(x) \in \{-1, +1, r\}$$

where r indicates abstaining from a prediction. This method is sometimes called **selective classification**. We also introduce a cost $c \in [0, 0.5]$ for abstaining. The loss becomes:

$$l(f(x), y) = \mathbf{1}_{f(x) \neq y} \mathbf{1}_{f(x) \neq r} + c \mathbf{1}_{f(x) = r}$$

We should abstain if:

$$c < \min\{p(x), 1 - p(x)\}$$

17 Classification

The margin of a decision hyperplane to be the (smallest) distance between the hyperplane and the data points. The margin of the hyperplane \hat{w} is defined as $\frac{1}{\|\hat{w}\|}$.

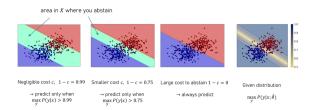


Figure 7: Asymmetric 0-1 Loss with Abstention

18 Quiz

18.1 K-means clustering

- Seeks cluster centers and assignments to minimize the within-cluster sum of squares.
- Appropriate if the underlying clusters are separable, spherical, and approximately of the same size.
- K-means clustering can be kernelized.

18.2 Find k

- By using a heuristic like the elbow method that identifies the diminishing returns from increasing k.
- By using an information criterion that regularizes the solution to favor simpler models with lower k.

18.3 Lloyd's algorithm

- It cannot cycle; i.e., it does never return to a particular solution after having previously changed to a different solution.
- Using specialized initialization schemes (e.g., k-means++) can improve the quality of solutions found by the algorithm and reduce its runtime.
- Center of clusters should be at the center of gravity.
- So after choosing centers and clustering, move centers to new centers.
- Repeat until done.
- Converges, local or global minimum.

18.4 PCA

- PCA can be kernelized.
- Unsupervised learning algorithm.
- It is orthogonal to all other principal components found by PCA.
- If we use the Gaussian kernel for kernel PCA, we implicitly perform PCA on an infinite-dimensional feature space.
- Gaussian kernel has infinite dimensions.
- Autoencoders and PCA are the same thing if we choose the activation function $\varphi(\cdot)$.
- For every arbitrary finite dataset with two classes and distinct points, there exists a feature map ϕ , such that the dataset becomes linearly separable.
 - As long as it is finite with two datasets A, B to separate, one can literally define a feature map:

$$\phi(x) = \begin{cases} 1 & \text{if } x \in A \\ -1 & \text{otherwise} \end{cases}$$

18.5 PCA first principal component

- Captures the maximum amount of variance in the data among all possible linear combinations of the original features.
- Represents the direction in the data space along which the data exhibits the highest variability or spread.
- Orthogonal to all other subsequent principal components, meaning it is uncorrelated with them. This orthogonality property allows PCA to create uncorrelated features.
- The first principal component is given by the eigenvector of the data covariance matrix with the largest eigenvalue.