Machine Learning Study Guide

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Contents

1 Linear Algebra and Calculus

1.1 General Notation

A vector $x \in \mathbb{R}^n$ has n entries, and $x_i \in \mathbb{R}$ is the i-th entry:

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n \tag{1}$$

We denote a matrix $A \in \mathbb{R}^{m \times n}$ with m rows and n columns, and $A_{ij} \in \mathbb{R}$ is the entry in the i-th row and j-th column:

$$A = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & & \vdots \\ A_{m1} & \cdots & A_{mn} \end{pmatrix} \in \mathbb{R}^{m \times n} \tag{2}$$

Vectors can be viewed as a $n \times 1$ matrix.

1.1.1 Indentity Matrix

The identity matrix $I \in \mathbb{R}^{n \times n}$ is a square matrix with ones along the diagonal and zero everywhere else:

$$I = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} \tag{3}$$

For all matrices $A \in \mathbb{R}^{n \times n}$ we have $A \times I = I \times A = A$.

1.1.2 Diagonal Matrix

A diagonal matrix $D \in \mathbb{R}^{n \times n}$ is a square matrix with nonzero values along the diagonal and zero everywhere else:

$$D = \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & d_n \end{pmatrix} \tag{4}$$

The diagonal matrix D is also written as $\text{diag}(d_1, \ldots, d_n)$.

1.1.3 Orthogonal Matrix

Two vectors $x, y \in \mathbb{R}^n$ are orthogonal if $x^T y = 0$. A vector $x \in \mathbb{R}^n$ is normalized if $||x||_2 = 1$. A square matrix $U \in \mathbb{R}^{n \times n}$ is orthogonal if all its columns are orthogonal to each other and are normalized. Hence:

$$U^T U = I = U U^T \tag{5}$$

Hence the inverse of an orthogonal matrix is its transpose.m

1.2 Matrix Operations

1.2.1 Vector-Vector Products

Given two vectors x, $y \in \mathbb{R}^n$, the inner product is:

$$x^T y = \sum_{i=1}^{n} x_i y_i \in \mathbb{R} \tag{6}$$

The outer product for a vector $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ is:

$$xy^T = \begin{pmatrix} x_1 y_1 & \cdots & x_1 y_n \\ \vdots & \ddots & \vdots \\ x_m y_1 & \cdots & x_m y_n \end{pmatrix} \in \mathbb{R}^{m \times n} \tag{7}$$

1.2.2 Vector-Matrix Products

The product of a matrix $A \in \mathbb{R}^{m \times n}$ and vector $x \in \mathbb{R}^n$ is a vector $y = Ax \in \mathbb{R}^m$. If we write A by the rows, Ax is expressed as:

$$y = Ax = \begin{pmatrix} - \ a_1^T \ - \\ - \ a_2^T \ - \\ \vdots \\ - \ a_m^T \ - \end{pmatrix} x = \begin{pmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{pmatrix} \tag{8}$$

Here, the i-th entry of y is the inner product of the i-th row of A and x, $y_i = a_i^T x$. If we write A is column form:

$$y = Ax = \begin{pmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = a_1 x_1 + a_2 x_2 + \ldots + a_n x_n \tag{9}$$

Here, y is a linear combination of the columns of A, where the coefficients of the linear combination are given by the entries of x.

1.2.3 Matrix-Matrix Products

Given a matrix $A \in \succcurlyeq \times \ltimes$ and matrix $B \in \ltimes \times \shortmid$, we can define $C = AB$ as follows:

$$C = AB = \begin{pmatrix} a_1^T b_1 & a_1^T b_2 & \cdots & a_1^T b_p \\ a_2^T b_1 & a_2^T b_2 & \cdots & a_2^T b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b_1 & a_m^T b_2 & \cdots & a_m^T b_p \end{pmatrix} \tag{10}$$

Hence, each (i, j)-th entry of C is equal to the inner product of the i-th row of A and the j-th column of B. Compactly:

$$C_{ij} = a_i^T b_j = \sum_{k=1}^{n} a_{ik} b_{kj} \tag{11}$$

1.2.4 The Transpose

The transpose of a matrix $A \in \mathbb{R}^{m \times n}$ is $A^T \in \mathbb{R}^{n \times m}$ matrix whose entries are:

$$(A^T)_{ij} = A_{ji} \tag{12}$$

Properties of the transpose:

1. $(A^T)^T = A$
2. $(AB)^T = B^T A^T$
3. $(A + B)^T = A^T + B^T$

1.2.5 The Trace

The trace of a square matrix $A \in \mathbb{R}^{n \times m}$ is denoted $\text{tr}(A)$. It is the sum of diagonal elements in the matrix:

$$\text{tr}\, A = \sum_{i=1}^{n} A_{ii} \tag{13}$$

Properties of the trace:

1. For $A \in \mathbb{R}^{n \times n}$, $\text{tr}\, A = \text{tr}\, A^T$
2. For $A, B \in \mathbb{R}^{n \times n}$, $\text{tr}(A + B) = \text{tr}\, A + \text{tr}\, B$
3. For $A \in \mathbb{R}^{n \times n}$, $t \in \mathbb{R}$, $\text{tr}(tA) = t \cdot \text{tr}\, A$
4. For A, B such that AB is square, $\text{tr}\, AB = \text{tr}\, BA$
5. For A, B, C such that ABC is square, $\text{tr}\, ABC = \text{tr}\, BCA = \text{tr}\, CAB$, and so on

1.2.6 The Inverse

The inverse of a matrix A is noted A^{-1} and is the unique matrix such that:

$$A^{-1}A = I = AA^{-1} \tag{14}$$

Not all square matrices are invertible. In addition, assuming $A, B \in \mathbb{R}^{n \times n}$ are non-singular:

1. $(A^{-1})^{-1} = A$
2. $(AB)^{-1} = B^{-1}A^{-1}$
3. $(A^{-1})^T = (A^T)^{-1}$

1.2.7 The Determinant

The determinant of a square matrix $A \in \mathbb{R}^{n \times n}$, noted $|A|$ or $\det(A)$ is expressed recursively in terms of $A_{\setminus i, \setminus j}$, which is the matrix A without its i-th row and j-th column, as follows:

$$\det(A) = |A| = \sum_{j=1}^{n} (-1)^{i+j} A_{i,j} |A_{\setminus i, \setminus j}| \tag{15}$$

Remark that A is invertible if and only if $|A| \neq 0$. Also, $|AB| = |A||B|$ and $|A^T| = |A|$.

1.3 Matrix Properties

1.3.1 Norms

A norm of a vector x is any function $f : \mathbb{R}^n \to \mathbb{R}$ that satisfies 4 properties:

1. Non-negativity: For all $x \in \mathbb{R}^n$, $f(x) \geq 0$
2. Definiteness: $f(x) = 0$ if and only if $x = 0$
3. Homogeneity: For all $x \in \mathbb{R}^n$, $t \in \mathbb{R}$, $f(tx) = |t|f(x)$
4. Triangle Inequality: For all $x, y \in \mathbb{R}^n$, $f(x + y) \leq f(x) + f(y)$

However, most norms used come from the family of ℓ_p norms:

$$\ell_p = ||x||_p = \left(\sum_{i=1}^{n} x_i^p \right)^{\frac{1}{p}} \tag{16}$$

The p-norm is used in Holder's inequality. The Manhattan norm, used in LASSO regularization, is:

$$\ell_1 = ||x||_1 = \sum_{i=1}^{n} |x_i| \tag{17}$$

The euclidean norm, ℓ_2 is used in ridge regularization and distance measures:

$$\ell_2 = ||x||_2 = \sqrt{\sum_{i=1}^{n} x_i^2} \tag{18}$$

Finally, the infinity norm is used in uniform convergence:

$$\ell_\infty = ||x||_\infty = \max_i |x_i| \tag{19}$$

The Frobenius norm of a matrix is analogous to the ℓ_2 norm of a vector:

$$||A||_F = \sqrt{\sum_{ij} A_{ij}^2} \tag{20}$$

The dot product of two vectors can be expressed in terms of norms:

$$x^T y = ||x||_2 ||y||_2 \cos\theta \tag{21}$$

where θ is the angle between vectors x and y.

1.3.2 Linear Dependence and Rank

A set of vectors $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^m$ is linearly independent if no vector can be represented as a linear combination of the remaining vectors. Conversely, if one vector in the set can be represented as a linear combination of the remaining vectors, then the vectors are said to be linearly dependent. Formally, for scalar values $\alpha_1, \ldots, \alpha_{n-1} \in \mathbb{R}$:

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i \tag{22}$$

The rank of a given matrix A is noted $\text{rank}(A)$ and is the dimension of the vector space generated by its columns. This is equivalent to the maximum number of linearly independent columns of A. If $\text{rank}(A) = \min(m, n)$, then A is said to be full rank.m

1.3.3 Span, Range, and Nullspace

The span of a set of vectors $\{x_1, x_2, \ldots, x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, x_2, \ldots, x_n\}$. Formally,

$$\text{span}\left(\{x_1, \ldots x_n\}\right) = \left\{ v : v = \sum_{i=1}^{n} \alpha_i x_i, \quad \alpha_i \in \mathbb{R} \right\} \tag{23}$$

The projection of a vector $y \in \mathbb{R}^n$ onto the span of $\{x_1, x_2, \ldots, x_n\}$ is the vector $v \in \text{span}\left(\{x_1, \ldots x_n\}\right)$ such that v is as close as possible to y as measured by the euclidean norm:

$$\text{Proj}\left(y; \{x_1, \ldots x_n\}\right) = \text{argmin}_{v \in \text{span}(\{x_1, \ldots, x_n\})} \|y - v\|_2 \tag{24}$$

The range of a matrix $A \in \mathbb{R}^{m \times n}$ is the span of the columns of A:

$$\mathcal{R}(A) = \{v \in \mathbb{R}^m : v = Ax, x \in \mathbb{R}^n\} \tag{25}$$

The nullspace of a matrix $A \in \mathbb{R}^{m \times n}$ is the set of all vectors that equal 0 when multiplied by A:

$$\mathcal{N}(A) = \{x \in \mathbb{R}^n : Ax = 0\} \tag{26}$$

1.3.4 Symmetric Matrices

A square matrix $A \in \mathbb{R}^{n \times n}$ is symmetric if $A = A^T$. It is anti-symmetric if $A = -A^T$. For any matrix $A \in \mathbb{R}^{n \times n}$ the matrix $A + A^T$ is symmetric and the matrix $A - A^T$ is anti-symmetric. From this, any square matrix $A \in \mathbb{R}^{n \times n}$ can be represented as a sum of a symmetric matrix and an anti-symmetric matrix:

$$A = \underbrace{\frac{A + A^T}{2}}_{\text{Symmetric}} + \underbrace{\frac{A - A^T}{2}}_{\text{Antisymmetric}} \tag{27}$$

1.3.5 Positive Semidefinite Matrices

Given a square matrix $A \in \mathbb{R}^{n \times n}$ and a vector $x \in \mathbb{R}^n$, the scalar value $x^T A x$ is called the quadratic form:

$$x^T A x = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \tag{28}$$

A symmetric matrix A is:

1. Positive definite (PD) if for all nonzero vectors, $x^T A x > 0$
2. Positive semidefinite (PSD) if for all nonzero vectors, $x^T A x \geq 0$
3. Negative definite (ND) if for all nonzero vectors, $x^T A x < 0$
4. Negative semidefinite (NSD) if for all nonzero vectors, $x^T A x \leq 0$
5. Indefinite if it is neiter PSD nor NSD, i.e. if there exists a x_1, x_2 such that $x_1^T A x_1 > 0$ and $x_2^T A x_2 < 0$

Given any matrix $A \in \mathbb{R}^{m \times n}$, the gram matrix $G = A^T A$ is always PSD. If $m \geq n$ and A is full rank, then G is PD.

1.3.6 Eigendecomposition

Given a square matrix $A \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{C}$ is an eigenvalue of A and $v \in \mathbb{C}$ is the corresponding eigenvector if

$$Av = \lambda v, \quad v \neq 0 \tag{29}$$

The trace of A is equal to the sum of its eigenvalues:

$$\operatorname{tr} A = \sum_{i=1}^{n} \lambda_i \tag{30}$$

The determinant of A is equal to the product of its eigenvalues:

$$|A| = \prod_{i=1}^{n} \lambda_i \tag{31}$$

Suppose matrix A has n linearly independent eigenvectors $\{v_1, \ldots, v_n\}$ with corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$. Let V be a matrix with one eigenvalue per column: $V = [v_1, \ldots, v_n]$. Let $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$. Then the eigendecomposition of A is given by:

$$A = V \Lambda V^{-1} \tag{32}$$

For when A is symmetric, then the eigenvalues of A are real, the eigenvectors of A are orthonormal, and hence V is an orthogonal matrix (henceforth renamed U). Hence $A = U \Lambda U^T$. A matrix whose eigenvalues are all positive is called positive definite. A matrix whose eigenvalues are all positive or zero valued is called positive semidefinite. Likewise, if all eigenvalues are negative, the matrix is negative definite, and if all eigenvalues are negative or zero valued, it is negative semidefinite. In addition, assuming sorted eigenvalues, for the following optimization problem:

$$\max_{x \in \mathbb{R}^n} x^T A x \quad \text{subject to } \|x\|_2^2 = 1 \tag{33}$$

The solution is v_1 the eigenvector corresponding to λ_1. For the minimization problem:

$$\min_{x \in \mathbb{R}^n} x^T A x \quad \text{subject to } \|x\|_2^2 = 1 \tag{34}$$

the optimal solution for x is v_n, the eigenvector corresponding to eigenvalue λ_n.

1.3.7 Singlular Value Decomposition

The singular value decomposition provides a way to factorize a $m \times n$ matrix A into singular vectors and singular values. It is defined as:

$$A = U D V^T \tag{35}$$

Suppose $A \in \mathbb{R}^{m \times n}$ matrix. Then $U \in \mathbb{R}^{m \times m}$, $D \in \mathbb{R}^{m \times n}$, $V \in \mathbb{R}^{n \times n}$ matrices. The matricies U and V are orthogonal, and matrix D is diagonal. The elements along the diagonal of D are known as the singular values of matrix A. The columns of U are known as the left-singular vectors while the columns of V are the right-singular vectors. The left-singular vectors of A are the eigenvectors of AA^T. The right-singular vectors of A are the eigenvectors of $A^T A$. We can use SVD to partially generalize matrix inversion to nonsquare matrices.

1.3.8 The Moore-Penrose Pseudoinverse

Matrix inversion is not defined for matrices that are not square. Note that for nonsingular A:

$$AA^{-1}A = A \tag{36}$$

However, if the inverse is not defined, we seek to find a matrix A^+ such that:

$$AA^+A = A \tag{37}$$

The moore-penrose pseudoinverse A^+ is defined as follows:

$$A^+ = \lim_{\alpha \to 0}(A^TA + \alpha I)^{-1}A^T \tag{38}$$

Practical algorithms use the singular value decomposition of A such that:

$$A^+ = VD^+U^T \tag{39}$$

where U, D, V are from the SVD of A, and the pseudoinverse of D^+ is obtained by taking the reciprocal of the nonzero diagonal elements of D. If A has more columns than rows, then using the pseudoinverse to solve a linear equation $Ax = y$ provides one of many solutions, but provides $x = A^+y$ with minimal euclidean norm $||x||_2$. When A has more rows than columns, the pseudoinverse gives us the x for which Ax is as close as possible to y, i.e. minimizing $||Ax - y||_2$.

1.4 Matrix Calculus

1.4.1 The Gradient

Let $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ be a function and $A \in \mathbb{R}^{m \times n}$ be a matrix. The gradient of f with respect to A is a $m \times n$ matrix noted as $\nabla_A f(A)$ such that:

$$\nabla_A f(A) \in \mathbb{R}^{m \times n} = \begin{pmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_1} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{pmatrix} \tag{40}$$

Or compactly for each ij entry:

$$\nabla_A f(A)_{ij} = \frac{\partial f(A)}{\partial A_{ij}} \tag{41}$$

However, the gradient of a vector $x \in \mathbb{R}^n$ is:

$$\nabla_x f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{pmatrix} \tag{42}$$

1.4.2 The Hessian

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function and $x \in \mathbb{R}^n$ be a vector. The hessian of f with respect to x is a $n \times n$ symmetric matrix noted as $H = \nabla_x^2 f(x)$ such that:

$$\nabla_x^2 f(x) \in \mathbb{R}^{n \times n} = \begin{pmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{pmatrix} \tag{43}$$

Or compactly:

$$\nabla_x^2 f(x)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j} \tag{44}$$

Note that the hessian is only defined when $f(x)$ is real-valued.

1.4.3 Gradient Properties

For matrices A, B, C and vectors x, b:

1. $\nabla_x b^T x = b$
2. $\nabla_x x^T A x = 2Ax$ (if A symmetric)
3. $\nabla_x^2 x^T A x = 2A$ (if A symmetric)
4. $\nabla_A \text{tr}(AB) = B^T$
5. $\nabla_{A^T} f(A) = (\nabla_A f(A))^T$
6. $\nabla_A \text{tr}(ABA^T C) = CAB + C^T AB^T$
7. $\nabla_A |A| = |A|(A^{-1})^T$

2 Convex Optimization

2.1 Convexity

2.1.1 Convex Sets

A set C is convex if, for any $x, y \in C$ and $\alpha \in \mathbb{R}$ with $0 \leq \alpha \leq 1$, we have

$$\alpha x + (1 - \alpha) y \in C \tag{45}$$

This point is known as a convex combination of x and y.

2.1.2 Convex Functions

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if its domain $\mathcal{D}(f)$ is a convex set, and if, for all $x, y \in \mathcal{D}(f)$ and $\alpha \in \mathbb{R}$, $0 \leq \alpha \leq 1$, we have:

$$f(\alpha x + (1 - \alpha) y) \leq \alpha f(x) + (1 - \alpha) f(y) \tag{46}$$

A function is strictly convex if:

$$f(\alpha x + (1 - \alpha) y) < \alpha f(x) + (1 - \alpha) f(y) \tag{47}$$

2.1.3 First-Order Conditions

Suppose a function $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable, then f is convex if and only if $\mathcal{D}(f)$ is a convex set and for all $x, y \in \mathcal{D}(f)$ we have:

$$f(y) \geq f(x) + \nabla_x f(x)^T (y - x) \tag{48}$$

This is called the first-order approximation to the function f at point x. This is approximating f with its tangent line at point x. The first order condition for convexity says that f is convex if and only if the tangent line is a global underestimator of the function f. In other words, if we take our function and draw a tangent line at any point, then every point on this line will lie below the corresponding point on f.

2.1.4 Second-Order Conditions

Suppose a function $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable, i.e. the hessian $\nabla_x^2 f(x)$ is defined for all points x in the domain of f. Then f is convex if and only if $\mathcal{D}(f)$ is a convex set and its hessian is PSD:

$$\nabla_x^2 f(y) \succeq 0 \tag{49}$$

2.1.5 Jensen's Inequality

Suppose we start with the inequality in the basic definition of a convex function:

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha)f(y) \tag{50}$$

We can extend this to convex combinations of more than one point:

$$f\left(\sum_{i=1}^{k} \alpha_i x_i\right) \leq \sum_{i=1}^{k} \alpha_i f(x_i) \tag{51}$$

For $\sum_k \alpha = 1$ and all $\alpha \geq 0$. This can be extended to integrals:

$$f\left(\int p(x)x dx\right) \leq \int p(x)f(x)dx \tag{52}$$

For $\int p(x)dx = 1$ and $p(x) \geq 0 \forall x$. This implies $p(x)$ is a probability density, and we can write our inequality in terms of expectations:

$$f(\mathbf{E}[x]) \leq \mathbf{E}[f(x)] \tag{53}$$

And is known as Jensen's inequality.

2.1.6 Sublevel Sets

Given a convex function $f : \mathbb{R}^n \to \mathbb{R}$ and a real number $\alpha \in \mathbb{R}$, the α-sublevel set is:

$$\{x \in \mathcal{D}(f) : f(x) \leq \alpha\} \tag{54}$$

In other words, the α-sublevel set is the set of all points x such that $f(x) \leq \alpha$.

2.2 Convex Optimization

A convex optimization problem seeks to optimize a convex function f with respect to a variable x and possible constraints.

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array} \tag{55}$$

where f is a convex function, g_i are convex functions, and h_i are affine functions. The optimal value p^* is equal to the minimum possible value of the objective function in the feasible region:

$$p^\star = \min\{f(x) : g_i(x) \leq 0, i = 1, \ldots, m, h_i(x) = 0, i = 1, \ldots, p\} \tag{56}$$

The optimal point x^* is a point such that $f(x^*) = p^*$.

2.2.1 Global Optimality

A point x is locally optimal if it is feasible and if there exists some $R > 0$ such that all feasible points z with $||x - z||_2 \leq R$, satisfy $f(x) \leq f(z)$. This means that for x to be locally optimal, there exists no nerby points that have a lower objective value. A point x is globally optimal if it is feadible and for all feasible points z, $f(x) \leq f(z)$. For a convex optimization problem, all locally optimal points are globally optimal.

2.2.2 Gradient Descent

Using $\alpha \in \mathbb{R}$ as the learning rate, we can update a set of parameters θ with respect to minimizing a function f as follows:

$$\theta := \theta - \alpha \nabla f(\theta) \tag{57}$$

Stochastic gradient descent (SGD) is updating the parameter based on each training example, and batch gradient descent is on a batch of training examples.

2.2.3 Newton's Algorithm

Newton's algorithm is a numerical method using information from the second derivative to find θ such that $f'(\theta) = 0$.

$$\theta := \theta - \frac{f'(\theta)}{f''(\theta)} \tag{58}$$

For multidimensional parameters:

$$\theta := \theta - \alpha H^{-1} \nabla_\theta f(\theta) \tag{59}$$

Where H is the hessian matrix of second partial derivatives.

$$H_{ij} = \frac{\partial^2 f(\theta)}{\partial \theta_i \partial \theta_j} \tag{60}$$

2.3 Lagrange Duality and KKT Conditions

Generic differentiable convex optimization problems are of the form:

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array} \tag{61}$$

where $x \in \mathbb{R}^n$ is the optimization variable, $f : \mathbb{R}^n \to \mathbb{R}$ and $g_i : \mathbb{R}^n \to \mathbb{R}$ are differentiable convex functions, and $h_i : \mathbb{R}^n \to \mathbb{R}$ are affine functions.

2.3.1 The Lagrangian

Given a convex constrained minimization problem, the generalized lagrangian is a function $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ defined as:

$$\mathcal{L}(x, \alpha, \beta) = f(x) + \sum_{i=1}^{m} \alpha_i g_i(x) + \sum_{i=1}^{p} \beta_i h_i(x) \tag{62}$$

We refer to x as the primal variables of the Lagrangian. The α and β are refered to as the dual variables or lagrange multipliers. The key idea behind Lagrangian duality is for any convex optimization problem, there always exist settings of the dual variables such that the unconstrained minimum of the Lagrangian with respect to the primal variables (keeping the dual variables fixed) coincides with the solution of the original constrained minimization problem.

2.3.2 Primal and Dual Problems

The primal problem is:

$$\min_x \underbrace{\left[\max_{\alpha, \beta : \alpha_i \geq 0, \forall i} \mathcal{L}(x, \alpha, \beta) \right]}_{\theta_{\mathcal{P}(x)}} = \min_x \theta_{\mathcal{P}}(x) \tag{63}$$

Here, $\theta_{\mathcal{P}} : \mathbb{R}^n \to \mathbb{R}$ is the primal objective, and the right hand side is the primal problem. In addition, $p^* = \theta_{\mathcal{P}}(x^*)$ is the optimal value of the primal objective.
The dual problem is:

$$\max_{\alpha,\beta:\alpha_i \geq 0,\forall i} \underbrace{\left[\min_x \mathcal{L}(x,\alpha,\beta)\right]}_{\theta_{\mathcal{D}(x)}} = \max_{\alpha,\beta:\alpha_i \geq 0,\forall i} \theta_{\mathcal{D}}(x) \tag{64}$$

Here, $\theta_{\mathcal{D}} : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ is the dual objective, and the right hand side is the dual problem. In addition, $s^* = \theta_{\mathcal{D}}(\alpha^*, \beta^*)$ is the optimal value of the dual objective.

2.3.3 Strong and Weak Duality

Weak duality for any pair of primal and dual problems, with d^* the optimal objective value of the dual problem and p^* as the optimal objective value of the primal problem we have:

$$d^* \leq p^* \tag{65}$$

Strong duality is when for any pair of primal and dual problems which satisfy certain technical conditions called constraint qualifications, then:

$$d^* = p^* \tag{66}$$

2.3.4 Complementary Slackness

If strong duality holds, then $\alpha_i^* g(x_i^*) = 0$ for each $i = 1, \ldots, m$. This property is known as complementary slackness. This implies the following:

$$\alpha_i^* > 0 \Longrightarrow g_i\left(x^*\right) = 0 \tag{67}$$

$$g_i\left(x^*\right) < 0 \quad \Longrightarrow \quad \alpha_i^* = 0 \tag{68}$$

2.3.5 The KKT Conditions

Suppose that $x^* \in \mathbb{R}^n$, $\alpha^* \in \mathbb{R}^m$ and $\beta^* \in \mathcal{R}^p$ satisfy the following conditions:

1. Primal feasibility: $g_i(x^*) \leq 0$, for $i = 1, \ldots, m$ and $h_i(x^*) = 0$ for $i = 1, \ldots, p$
2. Dual feasibility: $\alpha_i^* \geq 0$ for $i = 1, \ldots, m$
3. Complementary slackness: $\alpha_i^* g_i(x^*) = 0$ for $i = 1, \ldots, m$
4. Lagrangian stationarity: $\nabla_x \mathcal{L}(x^*, \alpha^*, \beta^*) = \vec{0}$

Then x^* is primal optimal and (α^*, β^*) are dual optimal. Furthermore, if strong duality holds, then any primal optimal x^* and dual optimal (α^*, β^*) must satisfy the conditions 1 through 4. These conditions are known as the Karush-Kuhn-Tucker (KKT) conditions.

3 Probability and Statistics

3.1 Basics

The set of all possible outcomes of an experiment is known as the sample space and denoted by S. Any subset E of the sample space is known as an event. An event is a set consisting of possible outcomes of the experiment.

3.1.1 Axioms of Probability

For each event E, we denote $P(E)$ as the probability of event E occuring. $P(E)$ satisfies the following properties:

1. Every probability is between 0 and 1 included:

$$0 \leq P(E) \leq 1 \tag{69}$$

2. The probability that at least one event in the sample space will occur is 1:

$$P(S) = 1 \tag{70}$$

3. For any sequence of mutually exclusive events $E_1, \ldots, E_n$ we have:

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{i=1}^{n} P(E_i) \tag{71}$$

3.1.2 Permutation

A permutation is an arrangement of r objects from a pool of n objects, in a given order. The number of such arrangements is given by $P(n, r)$:

$$P(n, r) = \frac{n!}{(n-r)!} \tag{72}$$

3.1.3 Combination

A combination is an arrangement of r objects from a pool of n objects, where order does not matter. The number of such arrangements is given by $C(n, r)$:

$$C(n, r) = \frac{P(n, r)}{r!} = \frac{n!}{r!(n-r)!} \tag{73}$$

Note that for $0 \leq r \leq n$ we have $P(n, r) \geq C(n, r)$.

3.2 Conditional Probability

Let B be an event with non-zero probability, the conditional proability of any event A given B is:

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \tag{74}$$

3.2.1 Bayes Rule

For events A, B such that $P(B) > 0$, we have:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \tag{75}$$

From Bayes rule, we have:

$$P(A \cap B) = P(A|B)P(B) = P(A)P(B|A) \tag{76}$$

Let $\{A_i, i \in [1, n]\}$ be such that for all i, $A_i \neq \varnothing$. We say that $\{A_i\}$ is a partition if we have:

$$\forall i \neq j, A_i \cap A_j = \emptyset \quad \text{and} \quad \bigcup_{i=1}^{n} A_i = S \tag{77}$$

Remark that for any event B in the sample space, we have:

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i) \tag{78}$$

Let $\{A_i, i \in [1, n]\}$ be a partition of the sample space, we can extend bayes rule as:

$$P(A_k|B) = \frac{P(B|A_k)P(A_k)}{\sum_{i=1}^{n} P(B|A_i)P(A_i)} \tag{79}$$

3.2.2 Independence

Two events A and B are independent if and only if we have:

$$P(A \cap B) = P(A)P(B) \tag{80}$$

3.3 Random Variables

A random variable X is a function that maps every element in a sample space to a real line.

3.3.1 Cumulative Distribution Function (CDF)

The cumulative distribution function F, which is monotonically non-decreasing and is such that $\lim_{x\to-\infty} F(X) = 0$ and $\lim_{x\to\infty} F(X) = 1$ is defined as:

$$F(x) = P(X \leq x) \tag{81}$$

In addition:

$$P(a < X \leq b) = F(b) - F(a) \tag{82}$$

3.3.2 Probability Density Function (PDF)

The probability density function is the derivative of the CDF. It has the following properties:

1. $f(x) \geq 0$
2. $\int_{-\infty}^{\infty} f(x) = 1$
3. $\int_{x\in A} f(x)dx = P(X \in A)$

3.3.3 Discrete PDF/CDF

If X is discrete, by denoting f as the PDF and F as the CDF, we have:

$$F(X) = \sum_{x_i \leq x} P(X = x_i) \tag{83}$$

$$f(x_j) = P(X = x_j) \tag{84}$$

And the following properties for the PDF:

$$0 \leq f(x_j) \leq 1 \tag{85}$$

$$\sum_{j} f(x_j) = 1 \tag{86}$$

3.3.4 Continuous PDF/CDF

If X is continuous, by denoting f as the PDF and F as the CDF, we have:

$$F(X) = \int_{-\infty}^{x} f(y)dy \tag{87}$$

$$f(x) = \frac{dF}{dx} \tag{88}$$

And the following properties for the PDF:

$$f(x) \geq 0 \tag{89}$$

$$\int_{-\infty}^{\infty} f(x)dx = 1 \tag{90}$$

3.3.5 Expectation

The expected value of a random variable, also known as the mean value or first moment, is denoted as $\mathbb{E}[X]$ or μ. It is the value obtained by averaging the results of a random variable. We use (D) for discrete, (C) for continuous.

$$\text{(D)} \quad \mathbb{E}[X] = \sum_{i=1}^{n} x_i f(x_i) \qquad \text{and} \quad \text{(C)} \quad \mathbb{E}[X] = \int_{-\infty}^{+\infty} xf(x)dx \tag{91}$$

The expected value of a function of a random variable $g(X)$ is:

$$\text{(D)} \quad \mathbb{E}[g(X)] = \sum_{i=1}^{n} g(x_i) f(x_i) \qquad \text{and} \quad \text{(C)} \quad \mathbb{E}[g(X)] = \int_{-\infty}^{+\infty} g(x)f(x)dx \tag{92}$$

The k-th moment, noted $\mathbb{E}[X^k]$ is the value of X^k that we expect to observe on average on infinitely many trials. The k-th moment is a case of the previous definition with $g : X \mapsto X^k$.

$$\text{(D)} \quad \mathbb{E}[X^k] = \sum_{i=1}^{n} x_i^k f(x_i) \qquad \text{and} \quad \text{(C)} \quad \mathbb{E}[X^k] = \int_{-\infty}^{+\infty} x^k f(x)dx \tag{93}$$

A characteristic function $\psi(\omega)$ is derived from a probability density function $f(x)$ and is defined as:

$$\text{(D)} \quad \psi(\omega) = \sum_{i=1}^{n} f(x_i) e^{i\omega x_i} \qquad \text{and} \quad \text{(C)} \quad \psi(\omega) = \int_{-\infty}^{+\infty} f(x)e^{i\omega x}dx \tag{94}$$

Remark that $e^{i\omega x} = \cos(\omega x) + i\sin(\omega x)$. The k-th moment can also be computed with the characteristic function as:

$$\mathbb{E}[X^k] = \frac{1}{i^k}\left[\frac{\partial^k \psi}{\partial \omega^k}\right]_{\omega=0} \tag{95}$$

3.3.6 Variance and Standard Deviation

The variance of a random variable, often noted $\text{Var}(X)$ or σ^2, is a measure of the spread of its distribution function. It is determined as follows:

$$\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2] = \mathbb{E}[X^2] - \mathbb{E}[X]^2 \tag{96}$$

The standard deviation of a random variable, often noted σ, is a measure of the spread of its distribution function which is compatible with the units of the actual random variable. It is determined as follows:

$$\sigma = \sqrt{\text{Var}[X]} \tag{97}$$

Note that the variance for any constant a is $\text{Var}[a] = 0$, and $\text{Var}[af(X)] = a^2\text{Var}[f(X)]$.

3.4 Discrete Random Variables

3.4.1 Bernoulli

For $X \sim Bernoulli(p)$, we define a binary event with a probability of p for a true event, and a false event with probability of $q = 1 - p$.

$$P(X = x) = \begin{cases} q = 1 - p & \text{if } x = 0 \\ p & \text{if } x = 1 \end{cases} \tag{98}$$

It can also be expressed as:

$$f(x; p) = p^k (1 - p)^{1-k} \quad \text{for } k \in \{0, 1\} \tag{99}$$

Other properties:

$$\mathbb{E}[X] = p \tag{100}$$

$$\text{Var}[X] = pq = p(1 - p) \tag{101}$$

$$\psi(\omega) = (1 - p) + pe^{i\omega} \tag{102}$$

3.4.2 Binomial

For $X \sim Binomial(n, p)$, the number of true events in n independent experiments, with true probability of p, false probability of $q = 1 - p$.

$$P(X = x) = \binom{n}{x} p^x (1 - p)^{n-x} \tag{103}$$

Other properties:

$$\mathbb{E}[X] = np \tag{104}$$

$$\text{Var}[X] = npq = np(1 - p) \tag{105}$$

$$\psi(\omega) = (pe^{i\omega} + (1 - p))^n \tag{106}$$

3.4.3 Geometric

For $X \sim Geometric(p)$, is the number of experiments with true probability of p until the first true event (number of trials to get one success).

$$P(X = x) = p(1 - p)^{x-1} \tag{107}$$

Other properties:

$$\mathbb{E}[X] = \frac{1}{p} \tag{108}$$

$$\text{Var}[X] = \frac{1 - p}{p^2} \tag{109}$$

$$\psi(\omega) = \frac{pe^{i\omega}}{1 - (1 - p)e^{i\omega}} \tag{110}$$

3.4.4 Poisson

For $X \sim Poisson(\lambda)$, for $\lambda > 0$, a probability distribution over the nonnegative integers used for modeling the frequency of rare events.

$$P(X = x) = \frac{\lambda^x}{x!} e^{-\lambda} \tag{111}$$

Other properties:

$$\mathbb{E}[X] = \lambda \tag{112}$$

$$\text{Var}[X] = \lambda \tag{113}$$

$$\psi(\omega) = e^{\lambda(e^{i\omega} - 1)} \tag{114}$$

3.5 Continuous Random Variables

3.5.1 Uniform

For $X \sim Uniform(a, b)$, we have equal probability density to every value between a and b.

$$f(x) = \begin{cases} \frac{1}{b-a} & \text{if } a \leq x \leq b \\ 0 & \text{otherwise} \end{cases} \tag{115}$$

Other properties:

$$\mathbb{E}[X] = \frac{a+b}{2} \tag{116}$$

$$\text{Var}[X] = \frac{(b-a)^2}{12} \tag{117}$$

$$\psi(\omega) = \frac{e^{i\omega b} - e^{i\omega a}}{(b-a)i\omega} \tag{118}$$

3.5.2 Exponential

For $X \sim Exponential(\lambda)$, $\lambda > 0$, is the decaying probability density over the nonnegative reals.

$$f(x) = \begin{cases} \lambda e^{-\lambda x} & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases} \tag{119}$$

Other properties:

$$\mathbb{E}[X] = \frac{1}{\lambda} \tag{120}$$

$$\text{Var}[X] = \frac{1}{\lambda^2} \tag{121}$$

$$\psi(\omega) = \frac{1}{1 - \frac{i\omega}{\lambda}} \tag{122}$$

3.5.3 Gaussian (Normal)

For $X \sim Normal(\mu, \sigma)$, denoted also $X \sim \mathcal{N}(\mu, \sigma)$.

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \tag{123}$$

Other properties:

$$\mathbb{E}[X] = \mu \tag{124}$$

$$\text{Var}[X] = \sigma^2 \tag{125}$$

$$\psi(\omega) = e^{i\omega\mu - \frac{1}{2}\omega^2\sigma^2} \tag{126}$$

3.6 Jointly Distributed Random Variables

The joint probability distribution of two random variables X and Y, denoted as f_{XY} is defined as:

$$\text{(D)} \quad f_{XY}(x_i, y_j) = P(X = x_i \text{ and } Y = y_j) \tag{127}$$

$$\text{(C)} \quad f_{XY}(x, y)\Delta x \Delta y = P(x \leqslant X \leqslant x + \Delta x \text{ and } y \leqslant Y \leqslant y + \Delta y) \tag{128}$$

Again, denote (D) as the discrete case, and (C) as the continuous case.

3.6.1 Marginal Density

The marginal density for a random variable X is:

$$\text{(D)} \quad f_X(x_i) = \sum_j f_{XY}(x_i, y_j) \qquad \text{and} \quad \text{(C)} \quad f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y)dy \tag{129}$$

3.6.2 Cumulative Distribution

The cumulative distribution F_{XY} is:

$$\text{(D)} \quad F_{XY}(x, y) = \sum_{x_i \leqslant x} \sum_{y_j \leqslant y} f_{XY}(x_i, y_j) \qquad \text{and} \quad \text{(C)} \quad F_{XY}(x, y) = \int_{-\infty}^{x} \int_{-\infty}^{y} f_{XY}(x', y')dx'dy' \tag{130}$$

3.6.3 Conditional Density

The conditional density of X with respect to Y, denoted $f_{X|Y}$ is defined as:

$$f_{X|Y} = \frac{f_{XY}(x, y)}{f_Y(y)} \tag{131}$$

3.6.4 Independence

Two random variables X and Y are independent if:

$$f_{XY}(x, y) = f_X(x) f_Y(y) \tag{132}$$

3.6.5 Expectation

Given two random variables X, Y and $g : \mathbb{R}^2 \to \mathbb{R}$ is a function of these two variables. Then the expected value of g is:

$$\text{(D)} \quad \mathbb{E}[g(X,Y)] = \sum_i \sum_j g(x_i, y_i) f(x_i, y_i) \qquad \text{and} \quad \text{(C)} \quad \mathbb{E}[g(X,Y)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x_i, y_i) f(x_i, y_i) dy dx \tag{133}$$

3.6.6 Covariance

The covariance of two random variables X and Y, denoted σ^2_{XY} or as $\text{Cov}[X, Y]$ is defined as:

$$\text{Cov}[X,Y] \triangleq \sigma^2_{XY} = \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] = \mathbb{E}[XY] - \mu_X \mu_Y \tag{134}$$

Where $\mu_X = \mathbb{E}[X]$ and $\mu_Y = \mathbb{E}[Y]$ respectively. If X and Y are independent, the covariance is 0.

$$\text{Var}[X + Y] = \text{Var}[X] + \text{Var}[Y] + 2\text{Cov}[X, Y] \tag{135}$$

3.6.7 Correlation

By noting σ_X, σ_Y as the standard deviations of X and Y, we define the correlation between the random variables X and Y as ρ_{XY}:

$$\rho_{XY} = \frac{\sigma^2_{XY}}{\sigma_X \sigma_Y} \tag{136}$$

Correlation for X, Y is $\rho_{XY} \in [-1, 1]$. If X, Y independent, then $\rho_{XY} = 0$

3.7 Parameter Estimation

3.7.1 Definitions

3.7.2 Bias

3.7.3 Mean and Central Limit Theorem

3.7.4 Variance

3.8 Probability Bounds and Inequalities

This section looks at various bounds that define how likely a random variable is to be close to its expectation.

3.8.1 Markov

Let $X \geq 0$ be a non-negative random variable. Then for all $a \geq 0$:

$$P(X \geq a) \leq \frac{\mathbb{E}[X]}{a} \tag{137}$$

3.8.2 Chebyshev

Let X be any random variable with finite expected value $\mu = \mathbb{E}[X]$ and finite non-zero variance σ^2. Then for all $k > 0$:

$$P(|X - \mathbb{E}[X]| \geq k\sigma) \leq \frac{1}{k^2} \tag{138}$$

3.8.3 Chernoff

Recall that the moment generating function for a random variable X is:

$$M_X(\lambda) := \mathbb{E}[e^{\lambda X}] \tag{139}$$

Then the chernoff bound for a random variable X, obtained by applying the markov inequality to $e^{\lambda X}$, for every $\lambda > 0$:

$$P(X \geq a) = P(e^{\lambda X} \geq e^{\lambda a}) \leq \frac{\mathbb{E}[e^{\lambda X}]}{e^{\lambda a}} \tag{140}$$

For the multiplicative chernoff bound, suppose $X_1, \ldots, X_n$ are independent random variables taking values in $\{0, 1\}$. Let X denote the sum, $\mu = \mathbb{E}[X]$ denote the sum's expected value. Then for any $0 < \delta < 1$,

$$P(X > (1+\delta)\mu) < \left(\frac{e^{\delta}}{(1+\delta)^{(1+\delta)}}\right)^{\mu} \leq e^{-\frac{\delta^2\mu}{3}} \tag{141}$$

$$P(X < (1-\delta)\mu) < \left(\frac{e^{-\delta}}{(1-\delta)^{(1-\delta)}}\right)^{\mu} \leq e^{-\frac{\delta^2\mu}{2}} \tag{142}$$

For $\delta \geq 0$,

$$P(X \geq (1+\delta)\mu) \leq e^{-\frac{\delta^2\mu}{2+\delta}} \tag{143}$$

$$P(X \leq (1-\delta)\mu) \leq e^{-\frac{\delta^2\mu}{2}} \tag{144}$$

3.8.4 Hoeffding

Let $X_1, \ldots, X_n$ be independent random variables such that $a_i \leq X_i \leq b_i$. The sum of these variables $S_n = \sum_i X_i$, then the Hoeffding inequality is:

$$P\left(S_n - \mathbb{E}\left[S_n\right] \geq t\right) \leq \exp\left(-\frac{2t^2}{\sum_i (b_i - a_i)^2}\right) \tag{145}$$

$$P\left(|S_n - \mathbb{E}\left[S_n\right]| \geq t\right) \leq 2\exp\left(-\frac{2t^2}{\sum_i (b_i - a_i)^2}\right) \tag{146}$$

The hoeffding lemma states that for a real-valued random variable X with expected value $\mathbb{E}[X] = 0$ and such that $a \leq X \leq b$, then for all $\lambda \in \mathbb{R}$ we have,

$$\mathbb{E}[e^{\lambda X}] \leq \exp\left(\frac{\lambda^2 (b-a)^2}{8}\right) \tag{147}$$

4 Information Theory

Information Theory revolves around quantifying how much information is present in a signal. The basic intuition lies in the fact that learning an unlikely event has occured is more informative than learning that a likely event has occured. The basics are:

1. Likely events should have low information content, and in the extreme case, events that are guaranteed to happen should have no information content whatsoever.
2. Less likely events should have higher information content.
3. Independent events should have additive information.

We satisfy all three properties by defining self-information of an event x for a probability distribution P as:

$$I(x) = -\log P(x) \tag{148}$$

We can quantify the amount of uncertainty in a distribution using Shannon entropy:

$$H(P) = \mathbb{E}_{\mathrm{x}\sim P}[I(x)] = -\mathbb{E}_{\mathrm{x}\sim P}[\log P(x)] \tag{149}$$

Which in the discrete setting is written as:

$$H(P) = -\sum_x P(x) \log P(x) \tag{150}$$

In other words, the Shannon entropy of a distribution is the expected amount of information in an event drawn from that distribution. It gives a lower bound on the number of bits needed on average to encode symbols drawn from a distribution P. If we have two separate probability distributions $P(x)$ and $Q(x)$ over the same random variable x, we can measure how different these two distributions are using the Kullback-Leibler (KL) divergence:

$$\begin{aligned} D_{\mathrm{KL}}(P\|Q) &= \mathbb{E}_{\mathbf{x}\sim P}\left[\log \frac{P(x)}{Q(x)}\right] \\ &= \mathbb{E}_{\mathbf{x}\sim P}\left[\log P(x) - \log Q(x)\right] \\ &= \sum_x P(x) \frac{\log P(x)}{\log Q(x)} \end{aligned} \tag{151}$$

In the case of discrete variables, it is the extra amount of information needed to send a message containing symbols drawn from probability distribution P, when we use a code that was designed to minimize the length of messages drawn from probability distribution Q. The KL divergence is always non-negative, and is 0 if and only if P and Q are the same. We can relate the KL divergence to cross-entropy.

$$\begin{aligned} H(P, Q) &= H(P) + D_{\mathrm{KL}}(P\|Q) \\ &= -\mathbb{E}_{\mathbf{x}\sim P}\left[\log Q(x)\right] \\ &= -\sum_x P(x) \log Q(x) \end{aligned} \tag{152}$$

Minimizing the cross-entropy with respect to Q is equivalent to minimizing the KL divergence, because Q does not participate in the omitted term (entropy is constant).

5 Learning Theory

5.1 Bias and Variance

5.2 Notation

5.2.1 Union Bound

5.2.2 Hoeffding Inequality For Bernoulli Variables

5.3 Training Error

For a given classifier h, we define the training error $\widehat{\epsilon}(h)$, also known as the empirical risk or empirical error, to be:

$$\widehat{\epsilon}(h) = \frac{1}{m}\sum_{i=1}^{m} 1_{\{h(x^{(i)}) \neq y^{(i)}\}} \tag{153}$$

5.4 Probably Approximately Correct (PAC)

PAC learning is a framework with the following set of assumptions:

5.5 Hypothesis Classes

5.5.1 Shattering

5.5.2 Upper Bound Theorem

5.5.3 VC Dimension

5.5.4 Vapnik Theorem

6 Linear Regression

Linear Regression seeks to approximate a real valued label y as a linear function of x:

$$h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \cdots + \theta_n \cdot x_n \tag{154}$$

The θ_i's are the parameters, or weights. If we include the intercept term via $x_0 = 1$, we can write our model more compactly as:

$$h(x) = \sum_{i=0}^{n} \theta_i \cdot x_i = \theta^T x \tag{155}$$

Here n is the number of input variables, or features. In Linear Regression, we seek to make $h(x)$ as close to y for a set of training examples. We define the cost function as:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m} \left(h\left(x^{(i)}\right) - y^{(i)}\right)^2 \tag{156}$$

6.1 LMS Algorithm

We seek to find a set of θ such that we minimize $J(\theta)$ via a search algorithm that starts at some initial guess for our parameters and takes incremental steps to make $J(\theta)$ smaller until convergence. This is know as gradient descent:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \tag{157}$$

Here, α is the learning rate. We can derive the partial derivative as:

$$\begin{aligned}\frac{\partial}{\partial\theta_j}J(\theta) &= \frac{\partial}{\partial\theta_j}\frac{1}{2}\left(h(x)-y\right)^2 \\ &= 2\cdot\frac{1}{2}\left(h(x)-y\right)\cdot\frac{\partial}{\partial\theta_j}(h(x)-y) \\ &= \left(h(x)-y\right)\cdot\frac{\partial}{\partial\theta_j}\left(\sum_{i=0}^{n}\theta_i x_i - y\right) \\ &= \left(h(x)-y\right)x_j\end{aligned} \tag{158}$$

Hence, for a single example (stochastic gradient descent):

$$\theta_j := \theta_j + \alpha\left(y^{(i)} - h\left(x^{(i)}\right)\right)x_j^{(i)} \tag{159}$$

This is called the LMS update rule. For a batched version, we can evaluate the gradient on a set of examples (batch gradient descent), or the full set (gradient descent).

$$\theta_j := \theta_j + \alpha\sum_{i=1}^{m}\left(y^{(i)} - h\left(x^{(i)}\right)\right)x_j^{(i)} \tag{160}$$

6.2 The Normal Equations

We can also directly minimize J without using an iterative algorithm. We define X as the matrix of all samples of size m by n. We let $\vec{y}$ be a m dimensional vector of all target values. We can define our cost function J as:

$$J(\theta) = \frac{1}{2}(X\theta-\vec{y})^T(X\theta-\vec{y}) = \frac{1}{2}\sum_{i=1}^{m}\left(h\left(x^{(i)}\right)-y^{(i)}\right)^2 \tag{161}$$

We then take the derivative and find its roots.

$$\begin{aligned}\nabla_\theta J(\theta) &= \nabla_\theta\frac{1}{2}(X\theta-\vec{y})^T(X\theta-\vec{y}) \\ &= \frac{1}{2}\nabla_\theta\left(\theta^TX^TX\theta - \theta^TX^T\vec{y} - \vec{y}^TX\theta + \vec{y}^T\vec{y}\right) \\ &= \frac{1}{2}\nabla_\theta\left(\operatorname{tr}\theta^TX^TX\theta - 2\operatorname{tr}\vec{y}^TX\theta\right) \\ &= \frac{1}{2}\left(X^TX\theta + X^TX\theta - 2X^T\vec{y}\right) \\ &= X^TX\theta - X^T\vec{y}\end{aligned} \tag{162}$$

To minimize J, we set its derivatives to zero, and obtain the normal equations:

$$X^TX\theta = X^T\vec{y} \tag{163}$$

Which solves θ for a value that minimizes $J(\theta)$ in closed form:

$$\theta = \left(X^TX\right)^{-1}X^T\vec{y} \tag{164}$$

6.3 Probabilistic Interpretation

Why does linear regression use the least-squares cost function? Assume that the target variables and inputs are related via:

$$y^{(i)} = \theta^T x^{(i)} + \epsilon^{(i)} \tag{165}$$

Here, $\epsilon^{(i)}$ is an error term for noise. We assume each $\epsilon^{(i)}$ is independently and identically distributed according to a Gaussian distribution with mean zero and some variance σ^2. Hence, $\epsilon^{(i)} \sim \mathcal{N}\left(0, \sigma^2\right)$, so the density for any sample $x^{(i)}$ with label $y^{(i)}$ is $y^{(i)}|x^{(i)}; \theta \sim \mathcal{N}\left(\theta^T x^{(i)}, \sigma^2\right)$. This implies:

$$p\left(y^{(i)}|x^{(i)}; \theta\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^T x^{(i)}\right)^2}{2\sigma^2}\right) \tag{166}$$

The probability of a dataset X is quantified by a likelihood function:

$$L(\theta) = L(\theta; X, \vec{y}) = p(\vec{y}|X; \theta) \tag{167}$$

Since we assume independence on each noise term (and samples), we can write the likelihood function as:

$$\begin{aligned} L(\theta) &= \prod_{i=1}^{m} p\left(y^{(i)}|x^{(i)}; \theta\right) \\ &= \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^T x^{(i)}\right)^2}{2\sigma^2}\right) \end{aligned} \tag{168}$$

To get the best choice of parameters θ, we perform maximum likelihood estimation such that $L(\theta)$ is maximized. Usually we take the negative log and minimize:

$$\begin{aligned} \ell(\theta) &= -\log L(\theta) \\ &= -\log \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^T x^{(i)}\right)^2}{2\sigma^2}\right) \\ &= -\sum_{i=1}^{m} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^T x^{(i)}\right)^2}{2\sigma^2}\right) \\ &= -m \log \frac{1}{\sqrt{2\pi}\sigma} + \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^T x^{(i)}\right)^2 \end{aligned} \tag{169}$$

Hence, maximizing $L(\theta)$ is the same as minimizing the negative log likelihood $\ell(\theta)$, which for linear regression is the least squares cost function:

$$\frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^T x^{(i)}\right)^2 \tag{170}$$

Under the previous probabilistic assumptions on the data, least-squares regression corresponds to finding the maximum likelihood estimate of θ. This is thus one set of assumptions under which least-squares regression can be justified as performing maximum likelihood estimation. Note that θ is independent of σ^2.

6.4 Locally Weighted Linear Regression

Locally Weighted Regression, also known as LWR, is a variant of linear regression that weights each training example in its cost function by $w^{(i)}(x)$, which is defined with parameter $\tau \in \mathbb{R}$ as:

$$w^{(i)}(x) = \exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2}\right) \tag{171}$$

Hence, in LWR, we do the following:

1. Fit θ to minimize $\sum_i w^{(i)} \left(y^{(i)} - \theta^T x^{(i)}\right)^2$
2. Output $\theta^T x$

This is a non-parametric algorithm, where non-parametric refers to the fact that the amount of information we need to represent the hypothesis h grows linearly with the size of the training set.

7 Logistic Regression

We can extend this learning to classification problems, where we have binary labels y that are either 0 or 1.

7.1 The Logistic Function

For logistic regression, our new hypothesis for estimating the class of a sample x is:

$$h(x) = g\left(\theta^T x\right) = \frac{1}{1 + e^{-\theta^T x}} \tag{172}$$

where $g(z)$ is the logistic or sigmoid function:

$$g(z) = \frac{1}{1 + e^{-z}} \tag{173}$$

The sigmoid function is bounded between 0 and 1, and tends towards 1 as $z \to \infty$. It tends towards 0 when $z \to -\infty$. A useful property of the sigmoid function is the form of its derivative:

$$\begin{aligned} g'(z) &= \frac{d}{dz}\frac{1}{1 + e^{-z}} \\ &= \frac{1}{\left(1 + e^{-z}\right)^2}\left(e^{-z}\right) \\ &= \frac{1}{\left(1 + e^{-z}\right)} \cdot \left(1 - \frac{1}{\left(1 + e^{-z}\right)}\right) \\ &= g(z)(1 - g(z)) \end{aligned} \tag{174}$$

7.2 Cost Function

To fit θ for a set of training examples, we assume that:

$$\begin{aligned} P(y = 1|x;\theta) &= h(x) \\ P(y = 0|x;\theta) &= 1 - h(x) \end{aligned} \tag{175}$$

This can be written more compactly as:

$$p(y|x;\theta) = (h(x))^y \left(1 - h(x)\right)^{1-y} \tag{176}$$

Assume m training examples generated independently, we define the likelihood function of the parameters as:

$$\begin{aligned} L(\theta) &= p\left(\vec{y}|X;\theta\right) \\ &= \prod_{i=1}^{m} p\left(y^{(i)}|x^{(i)};\theta\right) \\ &= \prod_{i=1}^{m} \left(h\left(x^{(i)}\right)\right)^{y^{(i)}} \left(1 - h\left(x^{(i)}\right)\right)^{1-y^{(i)}} \end{aligned} \tag{177}$$

And taking the negative log likelihood to minimize:

$$\begin{aligned} \ell(\theta) &= -\log L(\theta) \\ &= -\sum_{i=1}^{m} y^{(i)} \log h\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h\left(x^{(i)}\right)\right) \\ &= -\sum_{i=1}^{m} y^{(i)} \theta^T x^{(i)} - \log\left(1 + e^{\theta^T x^{(i)}}\right) \end{aligned} \tag{178}$$

This is known as the binary cross-entropy loss function.

7.3 Gradient Descent

Lets start by working with just one training example (x,y), and take derivatives to derive the stochastic gradient ascent rule:

$$\begin{aligned} \frac{\partial}{\partial \theta_j} \ell(\theta) &= -\left(y \frac{1}{g\left(\theta^T x\right)} - (1-y) \frac{1}{1 - g\left(\theta^T x\right)}\right) \frac{\partial}{\partial \theta_j} g\left(\theta^T x\right) \\ &= -\left(y \frac{1}{g\left(\theta^T x\right)} - (1-y) \frac{1}{1 - g\left(\theta^T x\right)}\right) g\left(\theta^T x\right)\left(1 - g\left(\theta^T x\right)\right) \frac{\partial}{\partial \theta_j} \theta^T x \\ &= -\left(y\left(1 - g\left(\theta^T x\right)\right) - (1-y) g\left(\theta^T x\right)\right) x_j \\ &= -\left(y - h(x)\right) x_j \end{aligned} \tag{179}$$

This therefore gives us the stochastic gradient ascent rule:

$$\theta_j := \theta_j + \alpha\left(y^{(i)} - h\left(x^{(i)}\right)\right) x_j^{(i)} \tag{180}$$

We must use gradient descent for logistic regression since there is no closed form solution for this problem.

7.4 Newton-Raphson Algorithm

The Hessian matrix for logistic regression is:

$$\frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta} = -\sum_{i=1}^{m} x^{(i)} x^{(i)T} \cdot h\left(x^{(i)}\right) \cdot \left(1 - h\left(x^{(i)}\right)\right) \tag{181}$$

Hence the second order update is:

$$\theta := \theta - \left(\frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta}\right)^{-1} \frac{\partial \ell(\theta)}{\partial \theta} \tag{182}$$

8 Softmax Regression

A softmax regression, also called a multiclass logistic regression, is used to generalize logistic regression when there are more than 2 outcome classes.

8.1 Softmax Function

The softmax function creates a probability distribution over a set of k classes for a training example x, with θ_k denoting the set of parameters to be optimzed for the k-th class.

$$p(y = k | x; \theta) = \frac{\exp\left(\theta_k^T x\right)}{\sum_j \exp\left(\theta_j^T x\right)} \tag{183}$$

8.2 MLE and Cost Function

We can write the maximum likelihood function for softmax regression as:

$$L(\theta) = \prod_{i=1}^{m} \prod_{k} p(y = k|x; \theta)^{\mathbf{1}\{y_i = k\}} \tag{184}$$

Where $\mathbf{1}\{y_i = k\}$ is the indicator function which is 1 if its argument is true, 0 otherwise. By taking the negative log likelihood:

$$\begin{aligned}
\ell(\theta) &= -\log L(\theta) \\
&= -\log \prod_{i=1}^{m} \prod_{k} p(y = k|x; \theta)^{\mathbf{1}\{y_i = k\}} \\
&= -\sum_{i=1}^{m} \sum_{k} \left(\mathbf{1}\{y_i = k\} \cdot \left(\theta_k^T x_i - \log \left(\sum_j \exp\left(\theta_j^T x_i\right) \right) \right) \right) \\
&= \sum_{i=1}^{m} -\theta_{y_i}^T x_i + \log \left(\sum_j \exp\left(\theta_j^T x_i\right) \right)
\end{aligned} \tag{185}$$

This is known as the cross-entropy loss function.

8.3 Gradient Descent

To perform gradient descent, we must take the derivative of our cost function, but it is important to note that the derivative for the correct class is different than the other classes.

$$\begin{aligned}
\nabla_{\theta_j} \ell(\theta) &= \nabla_{\theta_j} \left(\sum_{i=1}^{m} -\theta_{y_i}^T x_i + \log \left(\sum_k \exp\left(\theta_k^T x_i\right) \right) \right) \\
&= \sum_{i=1}^{m} \nabla_{\theta_j} \left(-\theta_{y_i}^T x_i \right) + \nabla_{\theta_j} \left(\log \left(\sum_k \exp\left(\theta_k^T x_i\right) \right) \right) \\
&= \sum_{i=1}^{m} \mathbf{1}\{y_i = j\} \cdot (-x_i) + \frac{\exp(\theta_j^T x_i)}{\sum_k \exp(\theta_k^T x_i)} \cdot x_i \\
&= \sum_{i=1}^{m} \left(\frac{\exp(\theta_j^T x_i)}{\sum_k \exp(\theta_k^T x_i)} - \mathbf{1}\{y_i = j\} \right) \cdot x_i
\end{aligned} \tag{186}$$

And our update equation for the j-th parameter weights is:

$$\theta_j := \theta_j - \alpha \left(\frac{\exp(\theta_j^T x_i)}{\sum_k \exp(\theta_k^T x_i)} - \mathbf{1}\{y_i = j\} \right) \cdot x_i \tag{187}$$

Note that since each class has a set of weights, our gradient is a matrix known as the jacobian $\mathbf{J}$, with k classes each with n feature weights.

$$\mathbf{J}_\theta = \begin{bmatrix} \frac{\partial \ell(\theta)}{\partial \theta_1} & \cdots & \frac{\partial \ell(\theta)}{\partial \theta_k} \end{bmatrix} = \begin{bmatrix} \frac{\partial \ell(\theta)}{\partial \theta_{11}} & \cdots & \frac{\partial \ell(\theta)}{\partial \theta_{k1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \ell(\theta)}{\partial \theta_{1n}} & \cdots & \frac{\partial \ell(\theta)}{\partial \theta_{kn}} \end{bmatrix} \tag{188}$$

9 Generalized Linear Models

9.1 Exponentional Family

9.2 Assumptions of GLMs

9.3 Examples

9.3.1 Ordinary Least Squares

9.3.2 Logistic Regression

9.3.3 Softmax Regression

10 Perceptron

11 Support Vector Machines

12 Margin Classification

13 Generative Learning: Gaussian Discriminant Analysis

A generative model learns who the data is generated by estimating $P(x|y)$ which is then used to estimate $P(y|x)$ via Bayes rule.

13.1 Assumptions

Gaussian Discriminant Analysis assumes the following:

1. $y \sim \text{Bernoulli}(\phi)$
2. $x|y=0 \sim \mathcal{N}(\mu_0, \Sigma)$
3. $x|y=1 \sim \mathcal{N}(\mu_1, \Sigma)$

Writing out the distributions be have:

$$P(y) = \phi^y \cdot (1-\phi)^{1-y} \tag{189}$$

$$P(x|y=k) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)\right) \tag{190}$$

13.2 Estimation

The log-likelihood of the data is given by:

$$\begin{aligned} \ell(\phi, \mu_0, \mu_1, \Sigma) &= \log \prod_{i=1}^{m} P(x^{(i)}, y^{(i)}; \phi, \mu_0, \mu_1, \Sigma) \\ &= \log \prod_{i=1}^{m} P(x^{(i)}|y^{(i)}; \phi, \mu_0, \mu_1, \Sigma) \cdot P(y^{(i)}; \phi) \end{aligned} \tag{191}$$

By maximizing ℓ with respect to the parameters, we get the following MLE of the parameters:

$$\phi = \frac{1}{m}\sum_{i=1}^{m} 1_{\{y^{(i)}=1\}} \tag{192}$$

$$\mu_k = \frac{\sum_{i=1}^{m} 1_{\{y^{(i)}=k\}} x^{(i)}}{\sum_{i=1}^{m} 1_{\{y^{(i)}=k\}}} \tag{193}$$

$$\Sigma = \frac{1}{m} \sum_{i=1}^{m} (x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T \tag{194}$$

13.3 Prediction

To classify a point x, we find the class $y = k$ which maximizes the probability:

$$\hat{y} = \arg\max_k P(y = k) \cdot \prod_j P(x_j | y = k) \tag{195}$$

14 Generative Learning: Naive Bayes

14.1 Assumptions

The naive bayes model supposes that the features of each data point are all independent:

$$P(x|y) = P(x_1, x_2, ..., x_n|y) = P(x_1|y)P(x_2|y)...P(x_n|y) = \prod_{i=1}^{n} P(x_i|y) \tag{196}$$

14.2 Estimation

We can write the likelihood of the data as:

$$\mathcal{L}(\phi_y, \phi_{j=l|y=k}) = \prod_{i=1}^{m} P(x^{(i)}, y^{(i)}) \tag{197}$$

with classes denoted by k and features $x_j = l$ (x_j takes on value l). By maximizing the estimates, we get:

$$\phi_y = P(y = k) = \frac{1}{m} \sum_{i=1}^{m} 1_{\{y^{(i)}=k\}} \tag{198}$$

$$\phi_{j=l|y=k} = P(x_j = l | y = k) = \frac{\sum_{i=1}^{m} 1_{\{y^{(i)}=k \wedge x_j^{(i)}=l\}}}{\sum_{i=1}^{m} 1_{\{y^{(i)}=k\}}} \tag{199}$$

14.2.1 Laplace Smoothing

Laplace smoothing allows for unseen data to have a probability, and not automatically destory the prediciton process by setting all classes to 0. We can replace our feature estimates with the following:

$$\phi_j = \frac{\sum_{i=1}^{m} 1_{\{x^{(i)}=j\}} + 1}{m + k} \tag{200}$$

Or more generically:

$$\phi_{j=l|y=k} = \frac{\sum_{i=1}^{m} 1_{\{x_j^{(i)}=l \wedge y^{(i)}=k\}} + 1}{\sum_{i=1}^{m} 1_{\{y^{(i)}=k\}} + |K|} \tag{201}$$

where $|K|$ is the number of classes

14.3 Prediction

To classify a point x, we find the class $y = k$ which maximizes the probability:

$$\hat{y} = \arg\max_k P(y = k) \cdot \prod_{i=j}^{n} P(x_j | y = k) \tag{202}$$

15 Tree-based Methods

15.1 Decision Trees

Decision Trees are created via the Classification and Regression Trees (CART) training algorithm. They can be represent as binary trees where at each node the partition the data space according to a threshold to minimize either gini impurity or entropy between the two child nodes.

15.2 Random Forest

Random forests are a tree-based technique that uses a high number of decision trees built out of randomly selected sets of features. Contrary to the simple decision tree, it is highly uninterpretable but its generally good performance makes it a popular algorithm. It averages the decisions across several trees to combat overfitting. Random forests are a type of ensemble methods.

15.3 Boosting

The idea of boosting methods is to combine several weak learners to form a stronger one. The main ones are summed up below:

1. Adaptive boosting: Known as adaboost, it places high weights on errors to improve at the next boosting step.
2. Gradient boosting: Weak learners are trained on the remaining errors.

Boosting requires training several models to improve upon previous ones.

16 K-Nearest Neighbors

The k-nearest neighbors algorithm, commonly known as k-NN, is a non-parametric approach where the response of a data point is determined by the nature of its k neighbors from the training set. It can be used in both classification and regression settings. The higher the parameter k, the higher the bias, and the lower the parameter k, the higher the variance.

16.1 Classification

In k-NN classification, the output is a class membership. An object is classified by a majority vote of its neighbors, with the object being assigned to the class most common among its k nearest neighbors (k is a positive integer, typically small). If $k = 1$, then the object is simply assigned to the class of that single nearest neighbor.

16.2 Regression

In k-NN regression, the output is the property value for the object. This value is the average of the values of its k nearest neighbors.

$$y = \frac{1}{k} \sum_{x_i \in \mathcal{N}_k(x)} y_i \tag{203}$$

where $\mathcal{N}_k(x)$ is the k nearest points around x.

17 K-Means Clustering

CLustering seeks to group similiar points of data together in a cluster. We denote $c^{(i)}$ as the cluster for data point i and μ_j as the center for cluster j. We denote k as the number of clusters and n as the dimension of our data.

17.1 Algorithm

After randomly initializing the cluster centroids $\mu_1, \mu_2, \ldots, \mu_k \in \mathbb{R}^n$, repeat until convergence:

1. For every data point i:
$$c^{(i)} = \arg\min_j ||x^{(i)} - \mu_j||^2 \tag{204}$$

2. For each cluster j:
$$\mu_j = \frac{\sum_{i=1}^{m} 1_{\{c^{(i)}=j\}} x^{(i)}}{\sum_{i=1}^{m} 1_{\{c^{(i)}=j\}}} \tag{205}$$

The first step is known as cluster assignment, and the second updates the cluster center (i.e. the average of all points in the cluster). In order to see if it converges, use the distortion function:

$$J(c, \mu) = \sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2 \tag{206}$$

The distortion function J is non-convex, and coordinate descent of J is not guaranteed to converge to the global minimum (i.e. susceptible to local optima).

17.2 Hierarchical Clustering

Hierarchical clustering is a clustering algorithm with an agglomerative hierarchical approach that builds nested clusters in a successive manner. The types are:

1. Ward Linkage: minimize within cluster distance
2. Average Linkage: minimize average distance between cluster pairs
3. Complete Linkage: minimize maximum distance between cluster pairs

17.3 Clustering Metrics

In an unsupervised learning setting, it is often hard to assess the performance of a model since we don't have the ground truth labels as was the case in the supervised learning setting.

Silhouette coefficient By noting a and b the mean distance between a sample and all other points in the same class, and between a sample and all other points in the next nearest cluster, the silhouette coefficient s for a single sample is defined as follows:

$$s = \frac{b - a}{\max(a, b)} \tag{207}$$

Calinskli-Harabaz Index By noting k the number of clusters, B_k and W_k the between and within-clustering dispersion matricies defined as:

$$B_k = \sum_{j=1}^{k} n_{c^{(i)}} (\mu_{c^{(i)}} - \mu)(\mu_{c^{(i)}} - \mu)^T \tag{208}$$

$$W_k = \sum_{i=1}^{m} (x^{(i)} - \mu_{c^{(i)}})(x^{(i)} - \mu_{c^{(i)}})^T \tag{209}$$

the Calinksli-Harabaz index $s(k)$ indicated how well a clustering model defines its clusters, such that higher scores indicate more dense and well separated cluster assignments. It is defined as:

$$s(k) = \frac{\text{Tr}(B_k)}{\text{Tr}(W_k)} \times \frac{N - k}{k - 1} \tag{210}$$

18 Expectation-Maximization

18.1 Mixture of Gaussians

18.2 Factor Analysis

19 Principal Component Analysis

Principal Component Analysis is a dimension reduction technique that finds the variance maximizing the directions onto which to project the data.

19.1 Eigenvalues, Eigenvectors, and the Spectral Theorem

Recall that for a given matrix $A \in \mathbb{R}^{n \times n}$, λ is said to be an eigenvalue of A if there exists a vector $z \in \mathbb{R}^n \backslash \{0\}$, called an eigenvector, such that:

$$Az = \lambda z \tag{211}$$

The spectral theorem states that given matrix $A \in \mathbb{R}^{n \times n}$, if A is symmetric then A is diagonalizable by a real orthogonal matrix $U \in \mathbb{R}^{n \times n}$. Note $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$. Then $\exists\, \Lambda$ such that:

$$A = U \Lambda U^T \tag{212}$$

Note that the eigenvector associated with the largest eigenvalue is called the principal eigenvector of matrix A.

19.2 Algorithm

The PCA procedure projects the data onto k dimensions by maximizing the variance of the data as follows:

1. Normalize the data to have mean 0, standard deviation 1:

$$x^{(i)} \leftarrow \frac{x^{(i)} - \mu}{\sigma} \tag{213}$$

where μ and σ^2 are:

$$\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)} \tag{214}$$

$$\sigma^2 = \frac{1}{m} \sum_{i=1}^{m} (x^{(i)} - \mu)^2 \tag{215}$$

2. Compute covariance matrix Σ, which is symmetric with real eigenvalues.

$$\Sigma = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}x^{(i)^T} \in \mathbb{R}^{n\times n} \tag{216}$$

3. Compute $u_1, \ldots, u_k \in \mathbb{R}^n$ the k orthogonal principal eigenvectors of Σ, i.e. the orthogonal eigenvectors of the k largest eigenvalues.

4. Project the data on $\text{span}_{\mathbb{R}}(u_1, ..., u_k)$ to create a vector $y^{(i)}$ from point $x^{(i)}$:

$$y^{(i)} = U^T x^{(i)} = \begin{pmatrix} u_1^T x^{(i)} \\ u_2^T x^{(i)} \\ \vdots \\ u_k^T x^{(i)} \end{pmatrix} \in \mathbb{R}^k \tag{217}$$

This procedure maximizes the variance among all k-dimensional spaces.

19.3 Algorithm: SVD

Eigenvalue decomposition is deifned for square matricies, and using the SVD of a data matrix X is often used in practice.

1. Zero-mean the data to have mean 0:

$$x^{(i)} \leftarrow x^{(i)} - \mu \tag{218}$$

   where μ is:

$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)} \tag{219}$$

2. Computed the singular value decomposition of X_μ, our zero-meaned data matrix:

$$X_\mu = USV \tag{220}$$

3. Take the first k columns of U as our transform matrix, denoted U_k.

4. Project the data to create a matrix Y from data matrix X_μ:

$$Y = XU_k \tag{221}$$

20 Independent Component Analysis

21 Reinforcement Learning

21.1 Markov Decision Processes

21.2 Policy and Value Functions

21.3 Value Iteration Algorithm

21.4 Q-Learning

22 Hidden Markov Models

23 Deep Learning: Basics

23.1 Basics

23.2 Activation Functions

23.3 Loss Functions

23.4 Backpropagation

23.5 Regularization Methods

23.6 Optimization Algorithms

23.7 Convolutional Networks

23.8 Recurrent Networks

Recurrent networks allow us to work with sequences, where x_t is the input at time t, h_t is the hidden state at time t, and h_{t-1} is the previous hidden state. RNNs allow us to propagate information through the hidden state h. Hidden states defualt to zero.

23.8.1 Elman RNN

The Elman RNN is the simplest layers, yet prone to both the vanishing and exploding gradient problem.

$$h_t = \tanh\left(W_{ih}x_t + b_{ih} + W_{hh}h_{t-1} + b_{hh}\right) \tag{222}$$

Here, W are weight matricies, and b are bias vectors, one each for the input and hidden vectors.

23.8.2 Long Short-Term Memory

LSTM RNNs mitigate the vanishing gradient problem. They involve a more complex set of equations corresponding to gates that control the amount of infomation to propagate through the sequence. Here, i is the input gate, f is the forget gate, g is the cell gate, and o is the output gate. LSTMs have two hidden inputs, hidden state h_t and

cell state c_t.

$$\begin{aligned} i_t &= \sigma\left(W_{ii}x_t + b_{ii} + W_{hi}h_{t-1} + b_{hi}\right) \\ f_t &= \sigma\left(W_{if}x_t + b_{if} + W_{hf}h_{t-1} + b_{hf}\right) \\ g_t &= \tanh\left(W_{ig}x_t + b_{ig} + W_{hg}h_{t-1} + b_{hg}\right) \\ o_t &= \sigma\left(W_{io}x_t + b_{io} + W_{ho}h_{t-1} + b_{ho}\right) \\ c_t &= f_t \circ c_{t-1} + i_t \circ g_t \\ h_t &= o_t \circ \tanh\left(c_t\right) \end{aligned} \tag{223}$$

Here, σ is the sigmoid function.

23.8.3 Gated Recurrent Unit

GRU RNNs are another rnn layer designed to mitigate the vanishing gradient problem. Here, we have the r reset gate, z update gate, and n is the new gate. σ is the sigmoid function.

$$\begin{aligned} r_t &= \sigma\left(W_{ir}x_t + b_{ir} + W_{hr}h_{t-1} + b_{hr}\right) \\ z_t &= \sigma\left(W_{iz}x_t + b_{iz} + W_{hz}h_{t-1} + b_{hz}\right) \\ n_t &= \tanh\left(W_{in}x_t + b_{in} + r_t \circ \left(W_{hn}h_{t-1} + b_{hn}\right)\right) \\ h_t &= (1 - z_t) \circ n_t + z_t \circ h_{t-1} \end{aligned} \tag{224}$$

23.8.4 Bidirectional RNNs

Bidirectional RNNs run two separate RNN layers on the forward and reverse sequence, and then concatenates them into one output vector.

$$\begin{aligned} \overrightarrow{h_f} &= \text{RNN}\left(\overrightarrow{x}\right) \\ \overleftarrow{h_r} &= \text{RNN}\left(\overleftarrow{x}\right) \\ h_o &= \left[\overrightarrow{h_f}\,;\, \overrightarrow{h_r}\right] \end{aligned} \tag{225}$$

Where RNN can be any of the 3 previously mentioned layers.

23.8.5 Vanishing/Exploding Gradient

The vanishing and exploding gradient phenomena are often encountered in the context of RNNs. The reason why they happen is that it is difficult to capture long term dependencies because of multiplicative gradient that can be exponentially decreasing/increasing with respect to the number of layers.

23.8.6 Gradient Clipping

Gradient clipping is a technique used to cope with the exploding gradient problem sometimes encountered when performing backpropagation. By capping the maximum value for the gradient, this phenomenon is controlled in practice.

$$\nabla\mathcal{L}_{clipped} = \min\left(\nabla\mathcal{L},\, C\right) \tag{226}$$

For some max value C.

24 Deep Learning: Advanced

24.1 Autoencoders

24.1.1 Variational Autoencoders

24.2 General Adversarial Networks

24.3 Encoder-Decoder Models

Encoder-decoder models allow for many to many RNN sequence learning. The idea for them is two take a source sequence, encode it to a vectorized output, and pass the hidden state over to the decoder (and possible the encodings themselves) to generate output. These models come up in machine tranlsations, allowing models to translate a source language into a target language.

24.3.1 Encoders

24.3.2 Decoders

24.4 Attention Models

Attention models were discussed by Bahdanau, and later Luong. They are a means to alter the representation of a set of encodings to pay attention to certain sequence elements more so than others. In an encoder-decoder model with out attention, the decoder relies exclusivly on the hidden state to hold all information. Attention, by contrast, uses the hidden state to create a context vector of the encodings.

24.4.1 Context Vector

Attention mechanisms rely on one simple concept: producing context vectors. Hence, given a set of encodeings $h = [h_i, \cdots, h_j, \cdots h_n]$ from the encoder, and the current hidden state s_{i-1}, we compute a score for each encoding h_j, denoted $score(s_{i-1}, h_j)$. These scores are discussed in later sections. With a score computed for each encoding, we apply a softmax across all scores:

$$a(s_{i-1}, h_j) = \frac{\exp(score(s_{i-1}, h_j))}{\sum_{j'} \exp(score(s_{i-1}, h_{j'}))} \tag{227}$$

These softmax proabilities are attention weights, and our context vector c_i is the weighted sum of the encodings given these weights:

$$c_i = \sum_{j'} a(s_{i-1}, h_{j'}) \cdot h_{j'} \tag{228}$$

These context vectors are appended to the embedding of the token set into the decoder.

24.4.2 Concat (Bahdanau) Attention

The concat attention scoring mechanism has two learnable weights, v_a and W_a and is defined as:

$$score(s_{i-1}, h_j) = v_a^T \cdot \tanh\left(W_a \cdot [s_{i-1}; h_j]\right) \tag{229}$$

24.4.3 Luong Attention Mechanisms

Luong defined several global attention mechanisms, defined here:

$$score(s_{i-1}, h_j) = \begin{cases} s_{i-1}^T \cdot W_a \cdot h_j & general \\ s_{i-1}^T \cdot h_j & dot \end{cases} \tag{230}$$

Luong also explored local attention weights, with monotonic alignment and predictive alignment. The difference in local attention is that the context vector is derived on source hidden states within the window $[p_t - D, p_t + D]$ for some D and decoder time step t (i.e. $i - 1$). In monotonic alignment, aligned position $p_t = t$. In predicitve alignment, the aligned position is:

$$p_t = S \cdot \sigma\left(v_p^T \tanh\left(W_p s_{i-1}\right)\right) \tag{231}$$

where v_p and W_p are learnable parameters, S is the source sentence length. In addition, the weights are gaussian centered around p_t:

$$a(s_{i-1}, h_j) = \frac{\exp(score(s_{i-1}, h_j))}{\sum_{j'} \exp(score(s_{i-1}, h_{j'}))} \cdot \exp\left(-\frac{(s - p_t)^2}{2\left(\frac{D}{2}\right)^2}\right) \tag{232}$$

Here, s is an integer within the window centered at p_t.

24.5 Word Embeddings

Word Embeddings seek to create a dense vector representation of real values to represent a single word in a euclidean space. Word vectors are weight matrices where each row corresponds to a word, acessed through a numerical token representing the word itself. However, several models have been developed to train these word embedding weights to encode lexical meaning.

24.5.1 N-Gram Models

A simple apporach is to take a context of size n words that appear before our target word, and attempt to train a model to predict a word w_i that appears in a training corpus. We effectively average the input word embeddings, apply a linear layer to project the data to the vocab size, and maximize the probability of predicitng the target word (i.e. apply a softmax of the output vector).

$$\max p(w_i \mid w_{i-n}, \ldots, w_{i-1}) = \max \frac{\exp f(w_{i-n}, \ldots, w_{i-1})_i}{\sum_{j=1}^{|V|} \exp f(w_{i-n}, \ldots, w_{i-1})_j} \tag{233}$$

Where our model is:

$$f(w_{i-n}, \ldots, w_{i-1}) = W_d \cdot \left(\frac{1}{n}\sum_{j=1}^{n} W_e[w_{i-j}]\right) + b_d \in \mathbb{R}^{|V|} \tag{234}$$

Here, $|V|$ is the size of the vocabulary, $W_d \in \mathbb{R}^{d \times |V|}$ is a projection matrix used for training along with bias b_d, and $W_e \in \mathbb{R}^{|V| \times d}$ are the word embeddings we seek to train. d is the embedding dimension.

24.5.2 Continuous Bag-of-Words Models (CBOW)

The continuous bag of words model, or CBOW, seeks to predict a center word given the surrounding context words.

24.5.3 Skip-Gram Model

24.5.4 Negative Sampling