ISSU0137 Machine Learning

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UCL Summer School Module Overview

Much of modern machine learning rests upon a range of mathematical methods and many introductory machine learning modules seek to introduce algorithms before ensuring the link with these methods is made. This module aims to offer students an introduction to traditional Machine Learning in a rigorous mathematical fashion. Assuming a familiarity with key results of Linear Algebra, Differential Calculus, Probability and Statistics, the module will introduce the key areas of traditional machine learning and will seek to cover the key tools (and theorems) within these areas, and to illustrate these with practical exemplars. The module will be delivered through a mixture of lectures and classes, and will involve a mix of traditional lecture delivery, interactive notebooks and problem sets.

Suggested Textbooks and Readings

- Deisenroth et al., Mathematics for Machine Learning
- Alpaydin, Introduction to Machine Learning (4th ed.)
- Bishop, Pattern Recognition and Machine Learning
- Lipschutz, Schaum's Outline of Linear Algebra
- Wrede & Spiegel, Schaum's Outline of Advanced Calculus
- Schiller at al., Schaum's Outline of Probability and Statistics
- Geron, Hands-On Machine Learning with Scikit-Learn, Keras, and Tensorflow (2nd ed.)

Contents

1 Linear Algebra

1.1 Linear Spaces & Linear Mappings

Vector Spaces

Definition (Addition and Scalar Multiplication)**.** To define a vector space, we define the operation on a set:

- An *addition* on a set V is a function $+ : (u, v) \in V^2 \mapsto u + v \in V$
- A *scalar multiplication* on a set V is a function $\times : (\lambda, v) \in \mathbb{F} \times V \mapsto \lambda v \in V$

Definition (Vector Space)**.** A set V equipped with addition and scalar multiplication on V satisfying the following properties:

- Commutative. $\forall u, v \in V$,
$$u + v = v + u$$
- Associative. $\forall u, v, w \in V$ and $\forall a, b \in \mathbb{F}$,
$$(u + v) + w = u + (v + w) \text{ and } (ab)w = a(bw).$$
- Additive Identity. $0 \in V$. $\forall v \in V$,
$$v + 0 = v$$
- Additive Inverse. $\forall v \in V, \exists!\, w \in V$,
$$v + w = 0.$$
- Multiplicative Identity. $1 \in \mathbb{F}$. $\forall v \in V$,
$$1v = v$$
- Distributive Properties. $\forall u, v \in V$ and $\forall a, b \in \mathbb{F}$,
$$a(u + v) = au + av \text{ and } (a + b)v = av + bv.$$

Satisfying these properties, we say that V is a vector space over $\mathbb{F}$.

In particular, we are interested in the *Euclidean Space* R^n. Vectors are hence n-tuples of real numbers defined as *column vectors*:
$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}.$$

Similarly, a *row vector* is defined as:
$$y^T = \left(y_1, y_2, \ldots, y_n\right).$$

The python library, numpy, can be used to encode a vector using *array* objects. We create a 3-dimensional column vector (in numpy a 3×1 array) as follows:

```python
x = np.array([1, 2, 3]) # [1 2 3]
x = x.reshape(-1, 1) # [[1]
                     #  [2]
                     #  [3]]
print(x.shape) # (3, 1)
```

To encode a row vector, we create a 2-dimensional 1×3 array as follows:

```python
y = np.array([[1, 2, 3]]) # [[1 2 3]
print(y.shape) # (1, 3)
```

Remark. With certain numpy functions we need to treat the vector as a 1-dimensional array. For this we use the `np.squeeze(x)` function.

Linear Independence, Span, Basis, Dimension

Definition (Linearly Independent)**.** A set of vectors $v_1, \dots, v_n \in \mathbb{V}$ is linearly independent $\iff$

$$a_1 v_1 + \cdots + a_n v_n = 0 \implies a_1 = \cdots = a_n = 0.$$

Definition (Span)**.** The span of $v_1, \dots, v_n \in \mathbb{V}$ is the set of all linear combinations vectors in $\mathbb{N}$

$$span(v_1, \dots, v_n) = \{\beta v_1 + \cdots + \beta v_n | \forall \beta_1, \dots, \beta_n \in \mathbb{R}\}.$$

Definition (Basis)**.** A basis for a vector space $\mathbb{V}$ is a set of linearly independent vectors which spans $\mathbb{V}$. The dimension of $\mathbb{V}$, $\dim(\mathbb{V})$ is the number of vectors in its bases.

Note that any vector $x \in \mathbb{V}$ can be expressed as a linear combination of a basis of $\mathbb{V}$.

Example (Standard Basis)**.** In particular, for any R^n, the standard basis is defined as:

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, e_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, e_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}.$$

Subspaces

Definition (Subspace)**.** A subset U of V that is also a vector space with the same additive identity, addition, and scalar multiplication as on V. We call U a *subspace* of V.

Proposition (Conditions for Subspace)**.** *A subset U of V is a subspace of V $\iff$ U satisfies the following conditions:*

- *Additive Identity: $0 \in U$.*
- *Closure under Addition: $u, w \in U \implies u + w \in U$.*
- *Closure under Scalar Multiplication: $a \in \mathbb{F} \wedge u \in U \implies au \in U$.*

Proof. If U is a subspace of V, U satifies the three conditions, by definition.
The first condition ensures the additive identity of V is in U. The second condition ensures that $+ : U \times U \mapsto U^2$ is defined. The third condition ensures that $\times : \mathbb{F} \times U \mapsto U$ is defined, and that the additive inverse of each element is in U. Associativity, commutativity and distributivity is inherited from V. Since U is a subset of V and is a vector space, it is a subspace of V, by definition.

Definition (Affine Subspaces)**.** For a vector space $\mathbb{V}$, a vector $x_0 \in \mathbb{V}$, a subspace $\mathbb{U} \subseteq \mathbb{V}$, $\mathbb{L}$ is an affine subspace or a linear manifold of $\mathbb{V}$ if:

$$\mathbb{L} = x_0 + \mathbb{U} = \{x_0 + u | u \in \mathbb{U}\}.$$

where

- $\mathbb{U}$ is the direction space
- x_0 is the support point

Example (Affine Subspaces)**.** For instance, any point, line or plane is an affine subspace of R^3.

Affine subspaces can be described by parameters: For a k-dimensional affine space $\mathbb{L}$ and a basis of $\mathbb{U}$, $\{x_1, x_2, \ldots, x_k\}$, every element $x \in \mathbb{L}$ can be described by parameters $\lambda_i \in \mathbb{R}$:

$$x = x_0 + \lambda_1 x_1 + \cdots + \lambda_k x_k.$$

Example (Hyperplanes)**.** In particular, hyperplanes are $(n-1)$-dimensional affine subspaces of R^n with elements $y \in \mathbb{R}^n$:

$$y = x_0 + \sum_{i=1}^{n-1} \lambda_i x_i.$$

where $\{\lambda_i\}_{i=1}^{n-1} \in \mathbb{R}, \mathbb{U} = span(x_1, x_2, \ldots, x_{n-1}) \subseteq \mathbb{R}^n$.

Matrices

Definition (Matrices)**.** A matrix $A \in \mathbb{R}^{n \times m}$ is an $n \times m$ array of numbers with elements $\{A_{ij}\}_{i,j=1}^{n,m}$:

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nm} \end{bmatrix}.$$

```
A=np.array([[1, 2],
            [4, 8],
            [3, 3]])
print(A.shape) # (3, 2)
```

Suppose finite-dimensional vector spaces $\mathbb{V}$ and $\mathbb{W}$ with bases $\{v_i\}_{i=1}^m$ and $\{w_i\}_{i=1}^n$ respectively. Then matrix $A \in \mathbb{R}^{n \times m}$ induces a linear map $f : \mathbb{R}^m \mapsto \mathbb{R}^n$ defined by:

$$f(x) = Ax$$

where $x \in \mathbb{V}, f(x) \in \mathbb{W}$
Some useful matrix operations and functions in numpy:

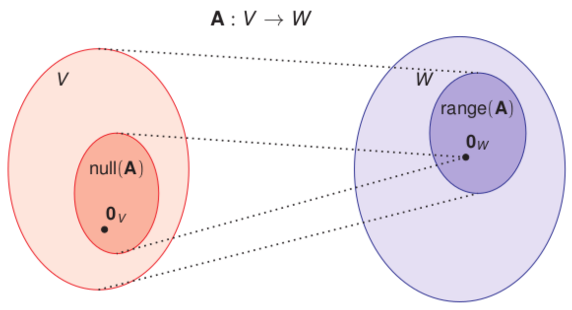
```python
# Matrix Addition
A = np.array([[1, 2],
              [4, 8],
              [3, 3]])
B = np.array([[4, 3],
              [6, 8],
              [8, 10]])
C = A + B

# Matrix Multiplication
A = np.array([[1, 2],
              [4, 8],
              [3, 3]])
B = np.array([[4, 3],
              [8, 10]])
C = np.matmul(A, B)

# Scalar Multiplication
A = np.array([[1, 2],
              [4, 8],
              [3, 3]])
a = 3
C = a*A
```

```python
# Transpose
A = np.array([[1, 2],
              [4, 8],
              [3, 3]])
A_t = np.transpose(A)

# Identity Matrix
A = np.array([[1, 2],
              [4, 8],
              [3, 3]])
I_n = np.eye(3)
I_m = np.identity(2)

# Inverse
def matrix_inverter(X):
    try:
        output = LA.inv(X)
    except LA.LinAlgError:
        output = None
    return output
A = np.array([[1, 2],
              [3, 3]])
A_inv = matrix_inverter(A)
```

Nullspace, Range, Columnspace, Rowspace, Rank, Nullity

Definition (Nullspace)**.** The nullspace, or kernel, or a linear map $A : \mathbb{V} \mapsto \mathbb{W}$ is:

$$null(A) = \{v \in V | Av = 0\}.$$



Definition (Range)**.** The range, or image, or A is:

$$range(A) = \{w \in \mathbb{W} | \exists v \in \mathbb{V}(Av = w)\}.$$

We can find possible bases for the range and nullspace of a matrix using SymPy:

```
A = np.array([[1, 2, 3],
              [4, 8, 12],
              [2, 8, 10],
              [3, 3, 6]])
mat_A = sy.Matrix(A)
print(str(sy.Matrix(A).columnspace()))
print(str(sy.Matrix(A).nullspace()))
```

Definition (Columnspace)**.** The columnspace of a matrix $A \in \mathbb{R}^{n \times m}$ is the span of the m columns.

$$C(A) = range(A).$$

Definition (Rowspace)**.** The rowspace of a matrix $A \in \mathbb{R}^{n \times m}$ is the span of the n rows.

$$R(A) = range(A^T).$$

```
A = np.array([[1, 2, 3],
              [4, 8, -1],
              [2, 8, 2],
              [3, 3, 0]])
mat_A = sy.Matrix(A)
```

Definition (Rank)**.** $rank(A) = \dim(C(A)) = \dim(R(A)) = \dim(range(A))$

Definition (Nullity)**.** $nullity(A) = \dim(null(A))$

Some results for the rank of a matrix:

- $rank(A) \leq \min(n, m)$
- $rank(AB) \leq rank(A)$
- $rank(AB) \leq \min(rank(A), rank(B))$

Theorem (Rank-Nullity Theorem)**.** $rank(A) + nullity(A) = m$

```
A = np.array([[1, 2, 3],
              [4, 8, -1],
              [2, 8, 2],
              [3, 3, 0]])
print('rank A = ' + str(LA.matrix_rank(A)))
print('rank A = ' + str(LA.matrix_rank(A)))
print('nullity A = ' + str(A.shape[1] - LA.matrix_rank(A)))
```

1.2 Geometrical Structure

Length, Similarity, Angle

To equip a vector space with a notion of length, we equip the vector space with a *norm*.

Definition (Norm)**.** A function on a real vector space $\mathbb{V}$, $\|\cdot\| : \mathbb{V} \mapsto \mathbb{R}$ for $\forall x, y \in \mathbb{V}, \forall \alpha \in \mathbb{R}$:

- $\|x\| \geq 0$, with equality $\iff x = 0$
- $\|\alpha x\| = |\alpha| \, \|x\|$
- $\|x + y\| \leq \|x\| + \|y\|$

Example (Norms)**.** We commonly define the l_p norm as follows:

$$\|x\|_p = (\sum_{i=1}^{n} |x_i|^p)^{\frac{1}{p}}.$$

In particular, we use the l_1, l_2 norms:

$$\|x\|_1 = \sum_{i=1}^{n} |x_i|.$$

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} (x_i)^2}.$$

```
x_vec = np.array([x_1, x_2]).reshape(-1,1)
l1_norm = LA.norm(x_vec, 1)
l2_norm = LA.norm(x_vec, 2)
```

To equip a vector space with a notion of similarity, we equip the vector space with a *inner product*.

Definition (Norm)**.** A function on a real vector space $\mathbb{V}$, $\langle \cdot, \cdot \rangle : \mathbb{V} \times \mathbb{V} \mapsto \mathbb{R}$ for $\forall x, y, z \in \mathbb{V}, \forall \alpha \in \mathbb{R}$:

- $\langle x, x \rangle \geq 0$ with equality $\iff x = 0$
- $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$
- $\langle \alpha x, y \rangle = \alpha \langle x, y \rangle$
- $\langle x, y \rangle = \langle y, x \rangle$

An inner product on $\mathbb{V}$ induces a norm on $\mathbb{V}$.

Example (Dot Product)**.** For Euclidean space the standard inner product is the *dot product*:

$$\langle x, y\rangle = x \cdot y = \sum_{i=1}^{n} x_i y_i = x^T y.$$

which induces the l_2 norm.

In addition, we define the notion of angle θ between two vectors $x, y \in \mathbb{V}$ via the dot product:

$$x \cdot y = \|x\|_2 \, \|y\|_2 \cos\theta.$$

```
x_vec = np.array([x_1, x_2]).reshape(-1,1)
y_vec = np.array([y_1, y_2]).reshape(-1,1)
l2_norm_x = LA.norm(x_vec, 2)
l2_norm_y = LA.norm(y_vec, 2)
dot_product = np.dot(np.squeeze(x_vec), np.squeeze(y_vec))
cos = dot_product/(l2_norm_x * l2_norm_y)
theta_deg = 360*np.arccos(cos)/(2 * mt.pi)
```

Orthonormality

Definition (Orthonormal)**.** Two vectors $x, y \in \mathbb{V}$ are said to be orthonormal if $\|x\|_1 = 1, \|y\|_1 = 1$ and they are orthogonal vectors (ie. $\langle x, y\rangle = 0$).

Definition (Orthogonal Matrix)**.** A square matrix $Q \in \mathbb{R}^{n\times n}$ is orthogonal if its columns are orthonormal:

$$Q^T = Q^{-1}.$$

Multiplication by an orthogonal matrix can be considered to be a mapping that preserves vector length while rotating or reflecting the vector about the origin.

$$(Qx) \cdot (Qy) = x \cdot y.$$

A rectangular matrix $\tilde{Q} \in \mathbb{R}^{n\times m}$ with orthonormal columns has a transpose that is the left inverse of itself:

$$\tilde{Q}^T \tilde{Q} = I_m \text{ but } \tilde{Q}\tilde{Q}^T \neq I_n.$$

Projections

Definition (Projection)**.** A projection $P_{\mathbb{U}} : \mathbb{V} \mapsto \mathbb{U}$ is a linear mapping from a vector space $\mathbb{V}$ to a subspace of $\mathbb{V}$, $\mathbb{U} \subseteq \mathbb{V}$ such that

$$P_{\mathbb{U}} P_{\mathbb{U}} = P_{\mathbb{U}} \implies P_{\mathbb{U}} P_{\mathbb{U}} v = P_{\mathbb{U}}$$

Example (Orthogonal Projections)**.** In Euclidean space, we consider orthogonal projections which map a vector $x \in \mathbb{R}^n$ to a vector $P_{\mathbb{U}} x \in \mathbb{U} \subseteq \mathbb{R}^n$ such that $\|x - P_{\mathbb{U}} x\|_2$ is minimised (it is closest to x). In other words, for a line $\overline{a} + t\overline{b}$, we seek a $P_{\mathbb{U}} \in \mathbb{R}^{n\times n}$ such that

- $P_{\mathbb{U}}x = \lambda b$ for some $\lambda \in \mathbb{R}$
- ${\|x - P_{\mathbb{U}}x\|_2}^2$ is minimal

Hence:

$$P_{\mathbb{U}} = \frac{bb^T}{{\|b\|_2}^2}.$$

Proof. We seek λ that satisfies:

$$\underset{\lambda}{\operatorname{argmin}} {\|x - \lambda b\|_2}^2.$$

Differentiating with respect to λ for stationary points yields:

$$2(x - \lambda b) \cdot b = 0 \implies \lambda = \frac{x \cdot b}{{\|b\|_2}^2}.$$

and that $(x - P_{\mathbb{U}}x)$ is orthogonal to b. Furthermore, we have:

$$P_{\mathbb{U}}x = \lambda b = b\lambda = b\frac{x \cdot b}{{\|b\|_2}^2} = b\frac{b^T x}{{\|b\|_2}^2} = \frac{bb^T}{{\|b\|_2}^2}x.$$

Example (Generalised Orthogonal Projections)**.** In general, for an m-dimensional subspace $\mathbb{U} \subseteq \mathbb{R}^n$ passing through the origin of basis vectors $\{b_i\}_{i=1}^m$:

- $P_{\mathbb{U}}x = \sum_{i=1}^m \lambda_i b^i = B\lambda$, where $B = [b_1, \ldots, b_m] \in \mathbb{R}^{n \times m}$
- ${\|x - P_{\mathbb{U}}x\|_2}^2$ is minimal

We seek λ satisfying:

$$\underset{\lambda}{\operatorname{argmin}} {\|x - B\lambda\|_2}^2.$$

Differentiating with respect to λ, $2B^T(x - B\lambda) = 0$ implies $(x - P_{\mathbb{U}}x)$ is orthogonal to b_i for all i, and

$$\lambda = {(B^T B)}^{-1} B^T x.$$

We have:

$$P_{\mathbb{U}} = B{(B^T B)}^{-1} B^T.$$

1.3 Linear Equations

One of the key uses of linear algebra is in the solution of systems of linear equations. For known $A \in \mathbb{R}^{n \times m}, b \in \mathbb{R}^n$ we would like to solve for an unknown $x \in R^m$ where

$$Ax = b.$$

This is equivalent to a set of n equations:

$$\begin{aligned} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1m}x_m &= b_1 \\ A_{21}x_1 + A_{22}x_2 + \cdots + A_{2m}x_m &= b_2 \\ &\vdots \\ A_{n1}x_1 + A_{n2}x_2 + \cdots + A_{nm}x_m &= b_n \end{aligned}$$

This system of equations can have a *unique solution*, *no solutions*, or *infinitely many solutions*, but it cannot have more than 1 and less than an infinite number of solutions.

1.4 Matrix Decomposition

Definition (Determinants)**.** Determinants are defined for square matrices only. For square matrix A, the determinant is denoted $\det(A)$ or $|A|$.

Example (For $\boldsymbol{A} \in \mathbb{R}^{\mathbf{2\times 2}}$)**.**

$$\det(A) = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = A_{11}A_{22} - A_{21}A_{12}.$$

Example (For $\boldsymbol{A} \in \mathbb{R}^{\mathbf{3\times 3}}$)**.**

$$\det(A) = \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = A_{11}\begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix} - A_{12}\begin{vmatrix} A_{21} & A_{23} \\ A_{31} & A_{33} \end{vmatrix} + A_{13}\begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix}.$$

Example (For $\boldsymbol{A} \in \mathbb{R}^{\boldsymbol{n\times n}}$)**.**

$$\det(A) = \sum_{j=1}^{n} (-1)^{i+j} A_{ij} \left|M_{ij}\right|.$$

Geometrically, the determinant is the signed volume of the n-dimensional paralleltope that results from the linear transform of A on the unit hypercube.

Remark. Some properties of the determinant:

- $\det(I) = 1$
- $\det(A^T) = \det(A)$
- $\det(AB) = \det(A)\det(B)$
- $\det(A^{-1}) = (\det(A))^{-1}$
- $\det(\alpha A) = \alpha^n \det(A)$

Definition (Traces)**.** Traces are defined for square matrices only. For square matrix $A \in \mathbb{R}^{n\times n}$, the trace is denoted $\operatorname{tr}(A) : \mathbb{R}^{n\times n} \mapsto \mathbb{R}$ and is defined as the sum of the diagonal elements of A:

$$\operatorname{tr}(A) = \sum_{i=1}^{n} A_{ii}.$$

Remark. Some properties of the trace:

- $\operatorname{tr}(A+B) = \operatorname{tr}(A) + \operatorname{tr}(B)$
- $\operatorname{tr}(\alpha A) = \alpha \operatorname{tr}(A)$
- $\operatorname{tr}(I_n) = n$
- $\operatorname{tr}(CD) = \operatorname{tr}(DC)$ for $C \in \mathbb{R}^{n\times k}, D \in \mathbb{R}^{k\times n}$

Matrix Decomposition

Definition (Singular Value Decomposition)**.** For any matrix $A \in \mathbb{R}^{n \times m}$,

$$\mathbf{A} = \mathbf{U\Sigma V^T}$$

where

- $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n]$ is an $n \times n$ orthogonal matrix, and $\mathbf{u}_i \in \mathbb{R}^n$ are known as left-singular vectors;
- $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m]$ is an $m \times m$ orthogonal matrix, and $\mathbf{v}_i \in \mathbb{R}^m$ are known as right-singular vectors;
- $\mathbf{\Sigma}$ is an $n \times m$ matrix with $\mathbf{\Sigma}_{ii} = \sigma_i \geq 0$, known as the singular values, and $\mathbf{\Sigma}_{ij} = 0, i \neq j$

To develop an intuition for the representation of SVD we consider the linear transform of the matrix A:

$$\mathbf{Ax} = \mathbf{U\Sigma V}^T\mathbf{x}.$$

There are three elements to this mapping:

- $\mathbf{x} \to \mathbf{Q}^T\mathbf{x}$ This represents a rotation of $\mathbf{x}$ in $\mathbb{R}^n$
- $(\mathbf{V}^T\mathbf{x}) \to \mathbf{\Sigma}(\mathbf{V}^T\mathbf{x})$ This represents a shear of $(\mathbf{V}^T\mathbf{x})$ in the axis-aligned directions and also adds rows of zeroes (if $m > n$) or deletes rows from it (if $n > m$)
- $(\mathbf{\Sigma V}^T\mathbf{x}) \to \mathbf{U}(\mathbf{\Sigma Q}^T\mathbf{x})$ This represents a rotation of $(\mathbf{\Lambda Q}^T\mathbf{x})$ inverse to the original rotation

Definition (Eigenvectors, Eigenvalues)**.** For a square matrix, $\mathbf{A} \in \mathbb{R}^{n \times n}$, we say that x is an eigenvector of A corresponding to an eigenvalue, λ, if:

$$Ax = \lambda x.$$

- This implies that: $(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}$
- Therefore if $(\mathbf{A} - \lambda\mathbf{I})^{-1}$ exists, then the unique solution is $\mathbf{x} = \mathbf{0}$
- Therefore for non-trivial solutions we must demand that $\nexists\ (\mathbf{A} - \lambda\mathbf{I})^{-1}$
- Therefore for non-trivial solutions $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$ [by the Invertible Matrix Theorem]
- $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$ is known as the characteristic polynomial of $\mathbf{A}$ and its (possibly non-unique) roots determine the possible eigenvalues of our problem

Definition (Eigendecomposition)**.** The eigendecomposition of a square matrix, $\mathbf{A} \in \mathbb{R}^{n \times n}$, with n linearly independent eigenvectors, $\{\mathbf{p}_i\}_{i=1}^n$ states that:

$$\mathbf{A} = \mathbf{P\Lambda P}^{-1}$$

where:

- $\mathbf{P} = [\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n]$;
- $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$

- λ_i is the eigenvalue associated with the eigenvector $\mathbf{q}_i$

It follows that:

$$\det(\mathbf{A}) = \prod_{i=1}^{n} \lambda_i$$

Note that such a decomposition does not exist for all matrices.

Symmetrical Matrix Decomposition

Definition (Spectral Decomposition)**.** For $\mathbf{A} \in \mathbb{R}^{n\times n}$ is (real and) symmetric, then there exists an orthonormal basis for $\mathbb{R}^n$ consisting of eigenvectors of $\mathbf{A}$, $\{\mathbf{q}_i | \mathbf{q}_i \cdot \mathbf{q}_j = \delta_{ij}, \quad \forall\, j\}_{i=1}^{n}$, and the associated eigenvalues are real. We call this particular eigendecomposition the spectral decomposition. From this it follows that the eigendecomposition of a real symmetric matrix, $\mathbf{A}$, is given by:

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$$

where:

- $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n]; \qquad \{\mathbf{q}_i | \mathbf{q}_i \cdot \mathbf{q}_j = \delta_{ij}, \quad \forall\, j\}_{i=1}^{n}$
- $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$
- λ_i is the eigenvalue associated with the eigenvector $\mathbf{q}_i$

To develop an intuition for the representation of the eigendecomposition we consider the linear transform of the matrix A:

$$\mathbf{A}\mathbf{x} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T\mathbf{x}.$$

There are three elements to this mapping:

- $\mathbf{x} \to \mathbf{Q}^T\mathbf{x}$ This represents a rotation of $\mathbf{x}$
- $(\mathbf{Q}^T\mathbf{x}) \to \mathbf{\Lambda}(\mathbf{Q}^T\mathbf{x})$ This represents a shear of $(\mathbf{Q}^T\mathbf{x})$ in axis-aligned directions
- $(\mathbf{\Lambda}\mathbf{Q}^T\mathbf{x}) \to \mathbf{Q}(\mathbf{\Lambda}\mathbf{Q}^T\mathbf{x})$ This represents a rotation of $(\mathbf{\Lambda}\mathbf{Q}^T\mathbf{x})$ inverse to the original rotation

1.5 Quadratic Forms

The quadratic form of a square matrix $\mathbf{M} \in \mathbb{R}^{n\times n}$ is defined:

$$\mathbf{x^T M x}.$$

Remark. It is always possile to express the quadratic form of a square matrix $\mathbf{M}$ as the quadratic form of an associated symmetric matrix $\mathbf{A} = \frac{1}{2}(\mathbf{M} + \mathbf{M^T})$:

$$\mathbf{x^T M x} = \mathbf{x^T A x}.$$

And since quadratic forms are scalars, $\mathbf{x^T M x} = \mathbf{x^T M^T x}$

Definiteness

A real symmetric matrix, $\mathbf{A}$, is said to be:

- Positive Semidefinite (psd), denoted $\mathbf{A} \succeq 0 \iff \mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0, \forall \mathbf{x} \neq \mathbf{0}$
- Positive Definite (pd), denoted $\mathbf{A} \succ 0 \iff \mathbf{x}^T\mathbf{A}\mathbf{x} > 0, \forall \mathbf{x} \neq \mathbf{0}$
- Negative Semidefinite (nsd), denoted $\mathbf{A} \preceq 0 \iff \mathbf{x}^T\mathbf{A}\mathbf{x} \leq 0, \forall \mathbf{x} \neq \mathbf{0}$
- Negative Definite (nd), denoted $\mathbf{A} \prec 0 \iff \mathbf{x}^T\mathbf{A}\mathbf{x} < 0, \forall \mathbf{x} \neq \mathbf{0}$
- Indefinite otherwise

Geometric Intepretation of PD Quadratic Forms

A function which occurs frequently in machine learning is:

$$f(\mathbf{x}) = \mathbf{x}^T\mathbf{A}\mathbf{x}$$

for some real, symmetric, positive definite $\mathbf{A}$. We are interested in the form of solutions to the following equation:

$$c = \mathbf{x}^T\mathbf{A}\mathbf{x}$$

for some constant c. We have the solution:

$$\mathbf{x} = \sqrt{c}\mathbf{Q}\mathbf{\Lambda}^{-\frac{1}{2}}\mathbf{z} \qquad \text{s.t. } \|\mathbf{z}\|_2 = 1$$

where:

- $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$
- $\mathbf{Q}$ is the matrix comprised of ordered orthonormal eigenvectors of $\mathbf{A}$
- $\mathbf{\Lambda}$ is the diagonal matrix of the ordered eigenvalues of $\mathbf{A}$
- $\mathbf{\Lambda}^{-\frac{1}{2}}$ is the diagonal matrix of the ordered inverse of the square root of the eigenvalues of $\mathbf{A}$

[N.B. The eigenvalues of $\mathbf{A}$ are all positive thus $\mathbf{\Lambda}^{-\frac{1}{2}}$ exists.]
The solution represents a mapping of three steps:

- Plot a circle of radius $\sqrt{c}$
- Apply a scaling mapping, $\mathbf{\Lambda}^{-\frac{1}{2}}$ to the circle, stretching by a factor equal to the inverse square root of the eigenvalues of $\mathbf{A}$ in each of the axis directions to form an axis-aligned ellipse
- Apply a rotation mapping, $\mathbf{Q}$ to the axis aligned ellipse, so that it is rotated such that the axes now line up with the eigenvectors of $\mathbf{A}$ to form an eigenvector-aligned ellipse

Our solution is hence an ellipsoid for which:

- The axes point in the direction of the eigenvectors of $\mathbf{A}$
- The radii are proportional to the inverse square root of the corresponding eigenvalues of $\mathbf{A}$

1.6 Important Results

Theorem (Invertible Matrix Theorem)**.** *For $A \in \mathbb{R}^{n\times n}$, the following statements are equivalent:*

- *A is invertible*
- $rank(A) = n$
- $\det(A) \neq 0$
- *The columns of A are linearly dependent*
- *The rows of A are linearly independent*
- $\nexists x (Ax = 0)$

Other useful results:

- $\mathbf{X^T X}$ is symmetric
- $\mathbf{X^T X} \succeq 0$
- $rank(\mathbf{X^T X}) = rank(\mathbf{X}) \leq \min(n, m)$
- $\exists (\mathbf{X^T X})^{-1} \iff (rank(\mathbf{X^T X}) = m) \iff \mathbf{X^T X} \succ 0$
- $rank(\mathbf{X^T X}) = rank(\mathbf{X^T X} | \mathbf{X^T y}), \forall \mathbf{y}$

2 Calculus

2.1 Derivatives

Definition (Derivatives)**.** A derivative defines a notion of continuous as follows:

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

It is the infinitessimal gradient at each particular point in the domain of a function.

Definition (Curvature)**.** The curvature of a function is the second-order derivative, a measure of how the gradient itself changes:

$$\frac{d^2 f}{dx^2} = f''(x) = \lim_{\delta \to 0} \frac{f'(x+\delta) - f'(x)}{\delta}.$$

Definition (Smoothness)**.** We say that a function is k-smooth $\iff$ the k-th-order derivative of the function is defined. If all higher order derivatives exist, the function is referred to as “smooth”.

Taylor Series

For small changes δ about a point $x = \tilde{x}$, any smooth function f can be approximated as an infinite polynomial expansion as follows:

$$f(\tilde{x} + \delta) = f(\tilde{x}) + \delta f'(\tilde{x}) + \frac{\delta^2}{2} f''(\tilde{x}) + \frac{\delta^3}{3!} f^{(3)}(\tilde{x}) + \dots$$

As the order of the taylor expansion increases, we approach the underlying function.

Taylor Expansion Results

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + \cdots = \sum_{n=0}^{\infty} x^n, |x| < 1.$$

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4 + \cdots = \sum_{n=0}^{\infty} \frac{1}{n!}x^n.$$

$$\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^{n+1}}{n}x^n, |x| < 1.$$

$$\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{24}x^{24} - \frac{1}{720}x^6 + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!}x^{2n}.$$

$$\sin(x) = x - \frac{1}{6}x^3 + \frac{1}{120}x^5 - \frac{1}{5040}x^7 + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!}x^{2n+1}.$$

2.2 Multivariate Calculus

Partial Derivatives, Gradients

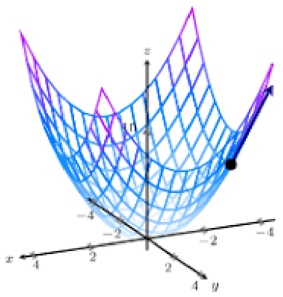
Definition (Partial Derivatives)**.** For a multivariate function $f : (x_1, x_2, \ldots, x_n) \mapsto f(x_1, \ldots, x_n)$ that depends on n variables, the partial derivative with respect to x_i is defined as:

$$\frac{\partial f}{\partial x_i} \lim_{\delta \to 0} = \frac{f(x_1, x_2, \ldots, x_i + \delta, \ldots, x_n) - f(x_1, x_2, \ldots, x_i, \ldots, x_n)}{\delta}.$$

Definition (Gradient Vectors)**.** We also use a vector for the set of partial derivatives for the function, the gradient vector defined as:

$$\nabla_x f = \begin{bmatrix} \frac{\partial f}{\partial x_i} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

Remark. The gradient vector is always perpendicular to the contour, and points in the direction of steepest ascent.



In addition, we can find the slope of $f(x)$ in a particular direction $\hat{u}$ for some $\|\hat{u}\|_2 = 1$. This is known as the directional derivative in the direction of $\hat{u}$:

$$\nabla_x f \cdot \hat{u} = \|\nabla_x f\|_2 \, \|\hat{u}\|_2 \cos\theta.$$

This directional derivative is maximal when $\theta = 0$, when $\hat{u}$ points in the direction of the gradient vector (used in gradient descent).

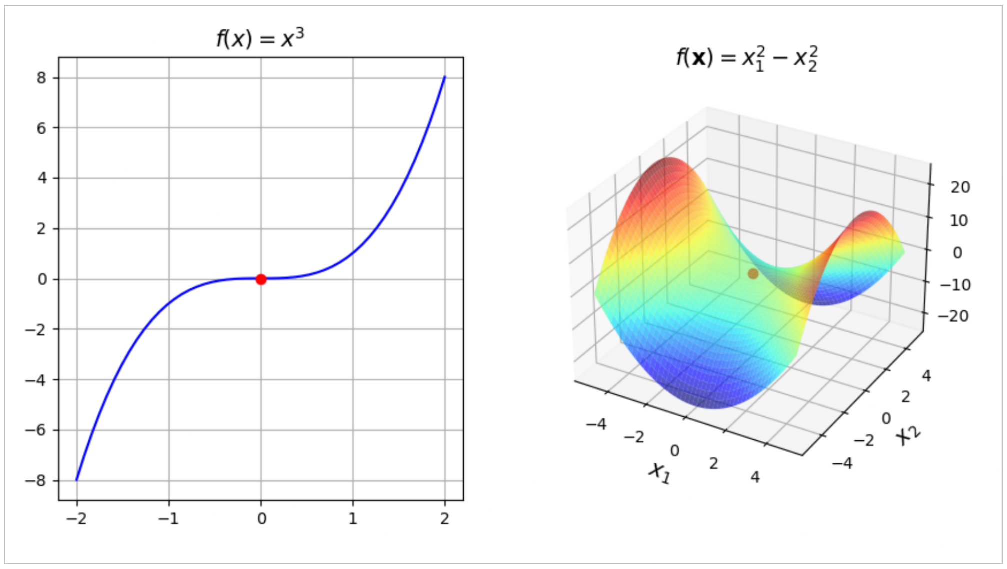
Stationary Points

Definition (Extrema)**.** For a function $f : \mathbb{R}^n \mapsto \mathbb{R}$ and a feasible set $X \subseteq \mathbb{R}^n$ over which we are optimising:

- A point x is a local minimum of f if $f(x) \leq f(y) \forall y \in N$ where $N \subseteq X$ is some neighbourhood about x.
- A point x is a global minimum of f in X if $f(x) \leq f(y) \forall y \in X$

It is a necessary condition that an extrema is stationary.

Definition (Saddle Points)**.** Any points for which $\nabla_x f = \mathbf{0}$ but where there is no local maximum or minimum are known as saddle points.



Hessian Matrix

To check whether particular critical points are maxima, minima or saddle points, we require information encoded in the second order derivatives.

Definition (Hessian Matrix)**.** We define the Hessian Matrix $\nabla_x^2 f$ or $H(x)$ as:

$$\nabla_x^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial {x_1}^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial {x_n}^2} \end{bmatrix}$$

Multivariate Taylor Series

We can equivalently express a multivariate function using an n-dimensional generalisation of the Taylor Series. For small $\boldsymbol{\delta}$ about a point $\mathbf{x} = \tilde{\mathbf{x}}$ in a 2-smooth function $f : \mathbb{F}^n \mapsto \mathbb{F}$:

$$f(\tilde{\mathbf{x}} + \delta) \approx f(\tilde{\mathbf{x}}) \boldsymbol{\delta}^T \nabla_x f(\tilde{\mathbf{x}}) + \frac{1}{2} \boldsymbol{\delta}^T \nabla_x^2 f(\tilde{\mathbf{x}}) \boldsymbol{\delta}.$$

Thus, at a critical point, we have (for sufficiently small $\boldsymbol{\delta}$):

$$f(\mathbf{x}^* + \delta) \approx f(\mathbf{x}^*) + \frac{1}{2}\boldsymbol{\delta}^T \nabla_x^2 f(\mathbf{x}^*)\boldsymbol{\delta}.$$

We have:

- $\mathcal{H}(\mathbf{x}^*) \succ 0$ then $f(\mathbf{x}^* + \boldsymbol{\delta}) > f(\mathbf{x}^*)$ for all $\boldsymbol{\delta} \implies \mathbf{x}^*$ is a local minimum.
- $\mathcal{H}(\mathbf{x}^*) \prec 0$ then $f(\mathbf{x}^* + \boldsymbol{\delta}) < f(\mathbf{x}^*)$ for all $\boldsymbol{\delta} \implies \mathbf{x}^*$ is a local maximum.
- $\mathcal{H}(\mathbf{x}^*)$ is indefinite $\implies f(\mathbf{x}^* + \boldsymbol{\delta}) > f(\mathbf{x}^*)$ in certain directions, while $f(\mathbf{x}^* + \boldsymbol{\delta}) < f(\mathbf{x}^*)$ in other directions $\implies \mathbf{x}^*$ is a saddle point.

2.3 Convexity

In performing optimisation, we are interested in discerning global extrema. This is hard in general, but for twice differentiable convex functions, it is more straightforward to do so.

Definition (Convex Set)**.** A set $\boldsymbol{\Omega}$ is convex if $\forall \mathbf{x}, \mathbf{y} \in \boldsymbol{\Omega}, \forall \theta \in [0,1], (\theta\mathbf{x} + (1-\theta)\mathbf{y} \in \boldsymbol{\Omega})$

Intuitively, if we take any two elements in $\boldsymbol{\Omega}$ and draw a line segment between the two elements, every point on that line segment belongs to $\boldsymbol{\Omega}$.

Definition (Convex Function)**.** A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if its domain is a convex set and if, $\forall \mathbf{x}_A, \mathbf{x}_B$ in its domain, and $\forall \lambda \in [0,1]$, we have:

$$f(\lambda\mathbf{x}_A + (1-\lambda)\mathbf{x}_B) \leq \lambda f(\mathbf{x}_A) + (1-\lambda)f(\mathbf{x}_B)$$

Definition (Strictly Convex Function)**.** A function $f : \mathbb{R}^n \to \mathbb{R}$ is strictly convex if its domain is a convex set and if, $\forall \mathbf{x}_A, \mathbf{x}_B$ in its domain, and $\forall \lambda \in (0,1)$, we have:

$$f(\lambda\mathbf{x}_A + (1-\lambda)\mathbf{x}_B) < \lambda f(\mathbf{x}_A) + (1-\lambda)f(\mathbf{x}_B)$$

Theorem (Sum of Convex Functions)**.** *If $f(\cdot)$ is a convex function, $g(\cdot)$ is a convex function, $h(\cdot)$ is a strictly convex function and $\alpha, \beta > 0$, then:*

- *$\alpha f(\cdot) + \beta g(\cdot)$ is a convex function.*
- *$\alpha f(\cdot) + \beta h(\cdot)$ is a strictly convex function.*

Theorem (Second Order Differential and Convexity)**.** *For 2-smooth f over an open domain:*

$$\nabla_{\mathbf{x}}^2 f(\mathbf{x}) \succeq 0 \quad \forall \mathbf{x} \in \mathit{dom}(f) \qquad \iff \qquad \textit{Convexity of } f$$

$$\nabla_{\mathbf{x}}^2 f(\mathbf{x}) \succ 0 \quad \forall \mathbf{x} \in \mathit{dom}(f) \qquad \implies \qquad \textit{Strict Convexity of } f$$

Global Optimality

Convexity is important in machine learning as it allows for the possibility to discern global extrema for such functions. For convex and differentiable f, any critical point is a globally optimal solution. Furthermore, for strictly convex f on a convex set $\boldsymbol{\Omega}$, the optimal solution is unique.

2.4 Quadratic Functions

Consider the following general quadratic function:

$$f(\mathbf{x}) = \mathbf{x}^{\mathbf{T}}\mathbf{A}\mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$$

for some $\mathbf{A} \in \mathbb{R}^{n \times n}, \mathbf{b} \in \mathbb{R}^n, c \in \mathbb{R}$, and variable $x \in \mathbb{R}^n$ WLOG we can re-write this as:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathbf{T}}\mathbf{B}\mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$$

for some symmetric $\mathbf{B} = (\mathbf{A} + \mathbf{A}^{\mathbf{T}})$.

Theorem (Convexity of Quadratic Functions)**.** *The convexity of a quadratic function is entirely determined by the definiteness of* $\mathbf{B}$*.*

$$\begin{aligned} \mathbf{B} \succeq 0 \quad &\iff \quad \textit{Convexity of } f \\ \mathbf{B} \succ 0 \quad &\iff \quad \textit{Strict Convexity of } f \end{aligned}$$

Optimisation of Quadratic Functions

Consider the unconstrained optimisation problem for some real symmetric $\mathbf{B}$:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathbf{T}}\mathbf{B}\mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c, \quad \min_{\mathbf{x}} f(\mathbf{x})$$

Parameters of f	Convexity of f	#	
$\mathbf{B} \succ 0$	Strictly Convex	1	$(\mathbf{B}\mathbf{x} = -\mathbf{b})$ consistent, exactly determined
$\mathbf{B} \succeq 0, \mathbf{B} \not\succ 0, \mathbf{b} \in range(\mathbf{B})$	Convex & Bounded Below	∞	$(\mathbf{B}\mathbf{x} = -\mathbf{b})$ consistent, underdetermined
$\mathbf{B} \succeq 0, \mathbf{B} \not\succ 0, \mathbf{b} \notin range(\mathbf{B})$	Convex & Unbounded Below	0	$(\mathbf{B}\mathbf{x} = -\mathbf{b})$ inconsistent
$\mathbf{B} \not\succeq 0$	Non-Convex	0	f unbounded below

3 Probability and Statistics

3.1 Probability Results and Concentration Inequalities

Some probability results:

- Principle of Inclusion Exclusion (PIE)

$$\begin{aligned} P(\bigcup_{i=1}^{n} E_i) = P(E_1 \cup E_2 \cup \ldots \cup E_n) = \sum_{i=1}^{n} P(E_i) - \sum_{i_1 < i_2} P(E_{i_1}E_{i_2}) + \ldots \\ + (-1)^{r+1} \sum_{i_1 < i_2 < \cdots < i_r} P(E_{i_1}E_{i_2} \ldots Ei_r) + \cdots + (-1)^{n+1} P(E_1E_2 \ldots E_n) \end{aligned}$$

- $$\begin{aligned} P(\bigcup_{i=1}^{n} E_i) &\leq \sum_{i=1}^{n} P(E_i) \\ &\geq \sum_{i=1}^{n} P(E_i) - \sum_{j<i} P(E_iE_j) \\ &\leq \sum_{i=1}^{n} P(E_i) - \sum_{j<i} P(E_iE_j) + \sum_{k<j<i} P(E_iE_jE_k) \end{aligned}$$

- $P(E_1E_2 \dots E_n) = P(E_1)P(E_2|E_1)\dots P(E_n|E_1 \dots E_{n-1})$
- For $F_1, F_2, \dots, F_n$ partitioning S,
$$P(E) = \sum_{i=1}^{n} P(EF_i) = \sum_{i=1}^{n} P(F_i)P(E|F_i)$$
- Baye's Theorem: E occurred. Which F_j most likely led to E:
$$\begin{aligned} P(F_j|E) &= \frac{P(EF_j)}{P(E)} = \frac{P(F_j)P(E|F_j)}{P(E)} \\ &= \frac{P(F_j)P(E|F_j)}{\sum_{i=1}^{n} P(F_i)P(E|F_i)} \end{aligned}$$
  $P(A)$ is known as the prior.
  $P(A|B)$ is known as the posterior.
  $P(B|A)$ is known as the likelihood.
  $P(B)$ is known as the evidence.
- Odds of $E = \frac{P(F)}{P(F^C)}$

Some concentration inequalities:

- Markov's Inequality [For non-negative $\mathcal{X}$ with expectation $E(X)$], $\forall a > 0$
$$P(X \geq 0) = 1 \Rightarrow P(X \geq a) \leq \frac{E(X)}{a}$$
- Chebyshev's Inequality [For finite $\mu, Var(X)$], $\forall k > 0$
$$P(|X - \mu| > k) \leq \frac{\sigma^2}{k^2}$$
- Hoeffding's Inequality [For i.i.d random variables $X_1, X_2, \dots$, such that each is bounded $[a_i, b_i]$, and let $\overline{\mathcal{X}}_n = \frac{1}{n}\sum_{i=1}^{n} \mathcal{X}_i$], $\forall \epsilon > 0$,
$$P(|\overline{\mathcal{X}} - E(\overline{\mathcal{X}})| \geq \epsilon) \leq 2\exp(-\frac{2n^2\epsilon^2}{\sum_{i=1}^{n}(b_i - a_i)^2})$$
$$P(\overline{\mathcal{X}} - E(\overline{\mathcal{X}}) \geq \epsilon) \leq \exp(-\frac{2n^2\epsilon^2}{\sum_{i=1}^{n}(b_i - a_i)^2})$$
- For i.i.d random variables $X_1, X_2, \dots$, $\forall \epsilon > 0$,
$$P(|\frac{X_1 + \cdots + X_n}{n} - \mu| \geq \epsilon) \to 0 \text{ as } n \to \infty$$
- For i.i.d $X_1, X_2, \dots$ where $E(X_i) = \mu, Var(X_i) = \sigma^2$,
$$\frac{X_1 + \cdots + X_n - n\mu}{\sigma\sqrt{n}} \sim N(0, 1) \text{ as } n \to \infty$$

3.2 Univariate Probability Distributions

Bernoulli Distribution

$\mathcal{X}$ is a discrete random variable, with outcomes, x, which can take one of two values: 0 or 1, with a probability that $x = 1$ being equal to θ

$$x \sim \text{Bern}(\theta)$$

$$p_{\mathcal{X}}(x;\theta) = \theta^x (1-\theta)^{1-x}$$

$$\mathbb{E}_{\mathcal{D}}[\mathcal{X}] = \theta$$

$$\text{Var}_{\mathcal{D}}[\mathcal{X}] = \theta(1-\theta)$$

Binomial Distribution

$\mathcal{X}$ is a discrete random variable, with outcomes, x, that denotes the number of successes, k, that we will achieve in n independent Bernoulli trials. $\mathcal{X}$ can be written as the sum of n independent Bernoulli trials $\{\mathcal{X}_i\}_{i=1}^n$, with outcomes $\{x_i \sim \text{Bern}(\theta)\}_{i=1}^n$:

$$\mathcal{X} = \mathcal{X}_1 + \mathcal{X}_2 + \cdots + \mathcal{X}_n$$

This characterises the associated $\mathcal{D}$ as a Binomial Distribution:

$$x \sim \text{Bin}(n,\theta)$$

$$p_{\mathcal{X}}(k;n,\theta) = \binom{n}{k} \theta^k (1-\theta)^{n-k}$$

$$\mathbb{E}_{\mathcal{D}}[\mathcal{X}] = n\theta$$

$$\text{Var}_{\mathcal{D}}[\mathcal{X}] = n\theta(1-\theta)$$

Beta Distribution

$\mathcal{X}$ be a continuous random variable, taking values $x \in [0,1]$, such that $\mathcal{D}$ follows a Beta distribution:

$$x \sim \text{Beta}(a,b) \qquad \text{where:} \qquad a,b > 0$$

This has a characteristic pdf $f_{\mathcal{X}}$:

$$f_{\mathcal{X}}(x;a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} x^{a-1}(1-x)^{b-1} \quad \text{where:} \quad \Gamma(a) = \int_0^\infty u^{a-1} e^{-u} du$$

$$\mathbb{E}_{\mathcal{D}}[\mathcal{X}] = \frac{a}{a+b}$$

$$\text{Var}_{\mathcal{D}}[\mathcal{X}] = \frac{ab}{(a+b)^2(a+b+1)}$$

Gaussian Distribution

$\mathcal{X}$ is a continuous random variable, taking values $x \in \mathbb{R}$, such that $\mathcal{D}$ follows a Gaussian distribution:

$$x \sim \mathcal{N}(\mu, \sigma^2) \qquad \text{where:} \qquad \mu \in \mathbb{R}, \sigma \in (0, \infty)$$

This has a characteristic pdf $f_{\mathcal{X}}$:

$$f_{\mathcal{X}}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

$$\mathbb{E}_{\mathcal{D}}[\mathcal{X}] = \mu$$

$$\text{Var}_{\mathcal{D}}[\mathcal{X}] = \sigma^2$$

3.3 Multivariate Probability Distribution

Covariance

Definition (Covariance)**.** The covariance is a measure of the linear relationship between two random variables, defined as:

$$\text{Cov}[\mathcal{X}_1, \mathcal{X}_2] = \mathbb{E}_{\mathcal{D}}\left[(\mathcal{X}_1 - \mathbb{E}_{\mathcal{D}_1}[\mathcal{X}_1])(\mathcal{X}_2 - \mathbb{E}_{\mathcal{D}_2}[\mathcal{X}_2])\right]$$

$$\text{Cov}[\mathcal{X}_1, \mathcal{X}_2] = \mathbb{E}_{\mathcal{D}}[\mathcal{X}_1\mathcal{X}_2] - \mathbb{E}_{\mathcal{D}_1}[\mathcal{X}_1]\,\mathbb{E}_{\mathcal{D}_2}[\mathcal{X}_2]$$

The covariance of some random vector, $\boldsymbol{\mathcal{X}} = [\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_m]^T$, with outcomes, $\mathbf{x} \sim \mathcal{D}$, where $\mathbf{x} = [x_1, x_2, \dots, x_m]^T$ and $\{x_i \sim \mathcal{D}_i\}_{i=1}^m$ is characterised by the covariance matrix:

$$\begin{aligned}\boldsymbol{\Sigma} &= \mathbb{E}_{\mathcal{D}}\left[(\boldsymbol{\mathcal{X}} - \mathbb{E}_{\mathcal{D}}[\boldsymbol{\mathcal{X}}])(\boldsymbol{\mathcal{X}} - \mathbb{E}_{\mathcal{D}}[\boldsymbol{\mathcal{X}}])^T\right] \\ &= \begin{bmatrix} \text{Var}[\mathcal{X}_1] & \text{Cov}[\mathcal{X}_1, \mathcal{X}_2] & \cdots & \text{Cov}[\mathcal{X}_1, \mathcal{X}_m] \\ \text{Cov}[\mathcal{X}_2, \mathcal{X}_1] & \text{Var}[\mathcal{X}_2] & \cdots & \text{Cov}[\mathcal{X}_2, \mathcal{X}_m] \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}[\mathcal{X}_m, \mathcal{X}_1] & \text{Cov}[\mathcal{X}_m, \mathcal{X}_2] & \cdots & \text{Var}[\mathcal{X}_m] \end{bmatrix}\end{aligned}$$

Remark. $\boldsymbol{\Sigma}$ is symmetric and positive semidefinite.

Definition (Correlation)**.** The correlation is the normalised covariance and always lies between -1 and 1:

$$\rho(\mathcal{X}_1, \mathcal{X}_2) = \frac{\text{Cov}[\mathcal{X}_1, \mathcal{X}_2]}{\sqrt{\text{Var}_{\mathcal{D}_1}[\mathcal{X}_1]\text{Var}_{\mathcal{D}_2}[\mathcal{X}_2]}}$$

We define a correlation matrix, a normalised version of the covariance matrix, to encode a set of correlations between m different random variables:

$$\boldsymbol{\rho} = \begin{bmatrix} 1 & \frac{\text{Cov}[\mathcal{X}_1,\mathcal{X}_2]}{\sqrt{\text{Var}_{\mathcal{D}_1}[\mathcal{X}_1]\text{Var}_{\mathcal{D}_2}[\mathcal{X}_2]}} & \cdots & \frac{\text{Cov}[\mathcal{X}_1,\mathcal{X}_m]}{\sqrt{\text{Var}_{\mathcal{D}_1}[\mathcal{X}_1]\text{Var}_{\mathcal{D}_m}[\mathcal{X}_m]}} \\ \frac{\text{Cov}[\mathcal{X}_2,\mathcal{X}_1]}{\sqrt{\text{Var}_{\mathcal{D}_2}[\mathcal{X}_2]\text{Var}_{\mathcal{D}_1}[\mathcal{X}_1]}} & 1 & \cdots & \frac{\text{Cov}[\mathcal{X}_2,\mathcal{X}_m]}{\sqrt{\text{Var}_{\mathcal{D}_2}[\mathcal{X}_2]\text{Var}_{\mathcal{D}_m}[\mathcal{X}_m]}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\text{Cov}[\mathcal{X}_m,\mathcal{X}_1]}{\sqrt{\text{Var}_{\mathcal{D}_m}[\mathcal{X}_m]\text{Var}_{\mathcal{D}_1}[\mathcal{X}_1]}} & \frac{\text{Cov}[\mathcal{X}_m,\mathcal{X}_2]}{\sqrt{\text{Var}_{\mathcal{D}_m}[\mathcal{X}_m]\text{Var}_{\mathcal{D}_2}[\mathcal{X}_2]}} & \cdots & 1 \end{bmatrix}$$

Multivariate Gaussian Distribution

A random vector $\boldsymbol{\mathcal{X}} = [\mathcal{X}_1, \dots, \mathcal{X}_n]^T$, with outcomes $\mathbf{x}$, has a multivariate Gaussian distribution if it has the following characterisation:

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad \text{where:} \qquad \boldsymbol{\mu} \in \mathbb{R}^n$$

The multivariate Gaussian has the characteristic pdf $f_{\boldsymbol{\mathcal{X}}}$:

$$f_{\boldsymbol{\mathcal{X}}}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{n/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right)$$

$$\mathbb{E}_{\mathcal{D}}[\boldsymbol{\mathcal{X}}] = \boldsymbol{\mu}$$

$$\mathrm{Cov}_{\mathcal{D}}[\boldsymbol{\mathcal{X}}] = \boldsymbol{\Sigma}$$

The isocontours of a multivariate Gaussian are characterised by the exponent of the pdf:

$$(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu})$$

which are ellipsoids:

- centred at $\boldsymbol{\mu}$
- with axes pointing in the direction of the eignevectors of $\boldsymbol{\Sigma}^{-1}$
- having radii proportional to the square root of the corresponding eigenvalues of $\boldsymbol{\Sigma}$

3.4 Maximum Likelihood Estimation

Likelihood

Suppose some random variable $\mathcal{X}$ the distribution of which $\mathcal{D}$ is parameterised by unknown variables $\theta \in \mathbb{R}^k$. Suppose we make a sequence of observations of outcomes $\mathcal{S}$ (itself an outcome of a random variable), and each i-th member x_i, is the outcome of the random variable $\mathcal{X}$.

Definition (Likelihood Function)**.** We define the likelihood function to be the joint probability function of a set of outcomes:

$$\mathbf{L}(\boldsymbol{\theta}) = p_{\S_1,\dots,\S_n}(x_1, \dots, x_n; \boldsymbol{\theta}).$$

This joint density is considered to be a function of $\boldsymbol{\theta}$.

Remark. The characterisation of the parameters θ being fixed but unknown is definitive of the **frequentist paradigm**.

Likelihood of i.i.d Random Variables

If the sequence of $\boldsymbol{\mathcal{X}}$ is i.i.d, we denote $\mathcal{S} \sim \mathcal{D}^n$, and the likelihood is expressed as:

$$\mathbf{L}(\boldsymbol{\theta}) = \prod_{i=1}^{n} p_{\S_i}(x_i; \boldsymbol{\theta}).$$

It is easier to optimise the logarithm of the likelihood function, and we define the log-likelihood:

$$\boldsymbol{\mathcal{L}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log\left(p_{\mathcal{X}_i}(x_i; \boldsymbol{\theta})\right).$$

Definition (Maximum Likelihood Estimate)**.** The MLE $\boldsymbol{\theta_{MLE}}$ is the value of $\boldsymbol{\theta}$ that maximises the likelihood function, i.e., the observed data is most probable with this parameterisation.

Notation ($\boldsymbol{\theta}^*$)*.* We define $\boldsymbol{\theta}^*$ to be the true unknown value of $\boldsymbol{\theta}$.

3.5 Maximum A Posteriori Estimation

The Maximum A Posteriori estimator is defined:

$$\theta_{MAP} = \underset{\theta}{\operatorname{argmax}} \left\{ p_{\Theta} \left(\theta | S \right) \right\}.$$

As n becomes large (as we gather more data), the prior distribution becomes less influential and the posterior becomes dominated by the likelihood function. i.e. as $n \to \infty$:

$$\theta_{MAP} \to \theta_{MLE} \quad \text{and} \quad \mu_{MAP} \to \mu_{MLE}.$$

4 Regression

4.1 Linear Regression

In Linear Regression we learn a mapping $\mathbf{f_w} : \mathbb{R}^m \mapsto \mathbb{R}$ between input attributes x and a single output y, drawn from a function class $\mathcal{F}$:

$$\mathcal{F} = \left\{ \mathbf{f_w}(\mathbf{X}) = \mathbf{w} \cdot \mathbf{x} | \mathbf{w} = [w_0, w_1, \dots, w_m]^T \in \mathbb{R}^{m+1} \right\}.$$

$\mathbf{f_w}$ is characterised by a weight vector $\mathbf{w}$ of which we define:

$$\mathbf{f_w}(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x}, \quad \mathbf{x} = [1, x_1, \dots, x_m]^T$$

Training Data

Suppose we draw n observations, each consisting m features (each i-th observation encoded $x^{(i)} \in \mathbb{R}^m$), as well as the output labels $y_i \in \mathbb{R}$. We represent our output training data as y:

$$\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}.$$

Definition (Design Matrix)**.** To represent the input attribute data more compactly, we define the design matrix X:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)T} \\ \mathbf{x}^{(2)T} \\ \vdots \\ \mathbf{x}^{(n)T} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_m^{(1)} \\ 1 & x_2^{(2)} & \cdots & x_m^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \cdots & x_m^{(n)} \end{bmatrix}.$$

We therefore seek $\mathbf{w}$ such that $\mathbf{y} = \mathbf{Xw}$. We have a solution only if $rank(\mathbf{X}) = rank(\mathbf{X}|\mathbf{y}) = (m+1) \leq n$. In general this is not true.

Evaluation

To make the problem well-defined, we choose an evaluation function to help us select the optimal weight vector. We consider the empirical squared error evaluation function:

$$L(\mathcal{E}, \mathcal{S}, \mathbf{f_w}) = \frac{1}{2n} \sum_{i=1}^{n} (y^{(i)} - \mathbf{w} \cdot \mathbf{x^{(i)}})^2.$$

We seek the $\mathbf{w}$ at which this evaluation function is minimised.

$$\mathbf{w}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}} \left(\frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \mathbf{w} \cdot \mathbf{x^{(i)}})^2 \right).$$

The optimal $\mathbf{w}_{OLS}$ is known as the Ordinary Least Squares estimator and this approach is known as OLS regression. Assuming the features and the output are related by an additive noise model:

$$y^{(i)} = \mathbf{w} \cdot \mathbf{x}^{(i)} + \epsilon^{(i)}.$$

The Gauss Markov Theorem demonstrates that $\mathbf{w}_{OLS}$ is the Best Linear Unbiased Estimator (BLUE). Further assuming the noise is normally distributed:

$$\epsilon \sim \mathcal{N}(0, \sigma^2) \quad \implies \quad \mathbf{y}|\mathbf{x} \sim \mathcal{N}(\mathbf{w} \cdot \mathbf{x}, \sigma^2)$$

The Maximum Likelihood Estimator $\mathbf{w}_{MLE}$ is:

$$\begin{aligned}
\mathbf{w}_{MLE} =& \underset{\mathbf{w}}{\operatorname{argmax}} \left\{ \ln \left(\prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{(y^{(i)} - w \cdot x^{(i)})^2}{2\sigma^2} \right) \right) \right\} \\
=& \underset{\mathbf{w}}{\operatorname{argmax}} \sum_{i=1}^{n} \ln \left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{(y^{(i)} - w \cdot x^{(i)})^2}{2\sigma^2} \right) \right) \\
=& \underset{\mathbf{w}}{\operatorname{argmax}} \left(-n \ln \sqrt{2\pi\sigma^2} - \sum_{i=1}^{n} \left(\frac{(y^{(i)} - w \cdot x^{(i)})^2}{2\sigma^2} \right) \right) \\
=& \underset{\mathbf{w}}{\operatorname{argmin}} \left(\frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(i)} \right)^2 \right) \\
=& \mathbf{w}_{OLS}
\end{aligned}$$

4.2 Linear Regression — Analytic Solution

Critical Points

We first find the gradient of the loss function:

$$
\begin{aligned}
L(\mathcal{E},\mathcal{S},f_w) =& \frac{1}{2n}\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2{}^2 \\
=& \frac{1}{2n}(\mathbf{y}-\mathbf{X}\mathbf{w})^{\mathbf{T}}(\mathbf{y}-\mathbf{X}\mathbf{w}) \\
\nabla_w L =& \frac{1}{2n}\nabla_w\left((\mathbf{y}-\mathbf{X}\mathbf{w})^{\mathbf{T}}(\mathbf{y}-\mathbf{X}\mathbf{w})\right) \\
=& \frac{1}{2n}\nabla_w\left(\mathbf{y}^{\mathbf{T}}\mathbf{y}-\mathbf{y}^{\mathbf{T}}\mathbf{X}\mathbf{w}-\mathbf{w}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{y}+\mathbf{w}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{X}\mathbf{w}\right) \\
=& \frac{1}{2n}\nabla_w\left(\mathbf{w}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{X}\mathbf{w}-\mathbf{2}\mathbf{y}^{\mathbf{T}}\mathbf{X}\mathbf{w}\right) \\
=& \frac{1}{n}\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\mathbf{w}-\mathbf{X}^{\mathbf{T}}\mathbf{y}\right)
\end{aligned}
$$

and solve for the criticial points of the function:

$$
\begin{aligned}
\nabla_w L =& 0 \\
0 =& \frac{1}{n}\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\mathbf{w}_{OLS}-\mathbf{X}^{\mathbf{T}}\mathbf{y}\right) \\
\mathbf{X}^{\mathbf{T}}\mathbf{X}\mathbf{w}_{OLS} =& \mathbf{X}^{\mathbf{T}}\mathbf{y}
\end{aligned}
$$

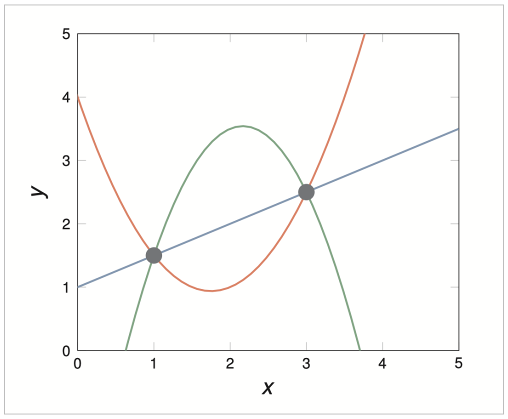
Since $rank(\mathbf{X}^{\mathbf{T}}\mathbf{X}) = rank(\mathbf{X}^{\mathbf{T}}\mathbf{X}|\mathbf{X}^{\mathbf{T}}\mathbf{y})$, the system is consistent and we have one or infinitely many solutions.
If $(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}$ exists we have the unique solution:

$$\mathbf{w}_{OLS} = (\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y}.$$

known as the **Normal Equations** with an analytic solution to the OLS approach.

- **Representation**
$$\mathcal{F} = \left\{\mathbf{w}\cdot\mathbf{x}|\mathbf{w}\in\mathbb{R}^{m+1}\right\}$$
- **Evaluation**
$$\frac{1}{2}\sum_{i=1}^{n}\left(y^{(i)}-\mathbf{w}\cdot\mathbf{x}^{(\mathbf{i})}\right)^2$$
- **Optimisation**
$$\mathbf{w}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}}\left\{\frac{1}{2}\sum_{i=1}^{n}\left(y^{(i)}-\mathbf{w}\cdot\mathbf{x}^{(\mathbf{i})}\right)^2\right\}$$

If $(\mathbf{X}^{\mathbf{T}}\mathbf{X})$ is non-invertible then $rank(\mathbf{X}^{\mathbf{T}}\mathbf{X}) < (m+1)$, the problem is undetermined and we have an infinite number of solutions. This is known as overfitting.



Optimality

To check for the optimality of the solution, we first obtain the Hessian:

$$\nabla_w^2 L = \mathbf{X^T X}$$

Since the Hessian matrix is positive semidefinite ($\mathbf{a^T X^T X a} = \|\mathbf{Xa}\|_\mathbf{2}{}^\mathbf{2} \geq 0 \quad \forall \mathbf{a} \in \mathbb{R}^{m+1}$), L is convex and a critical point is globally optimal

Uniqueness

Uniqueness of the solution requires that Hessian is positive definite $\iff$ $(\mathbf{X^T X})^{-1}$, such that the function is strictly convex. Otherwise, the function is not strictly convex (but still bounded since $\mathbf{X^T y} \in range(\mathbf{X^T X})$).

Remark. Matrix Derivation Results w.r.t. w:

- Linear form: $a^T w \implies \nabla_w(a^T w) = a$ for some constant vector a
- Quadratic form: $w^T A w \implies \nabla_w(w^T A w) = (A + A^T)w$for some constant matrix A

Limitations

The problem does not scale well with the dimensionality of the input attributes m. Matrix inversion requires $O(m^3)$ operations — which is expensive for large $\mathbf{X^T X}$. There are also space constraints for very high m to store $\mathbf{X^T X}$.

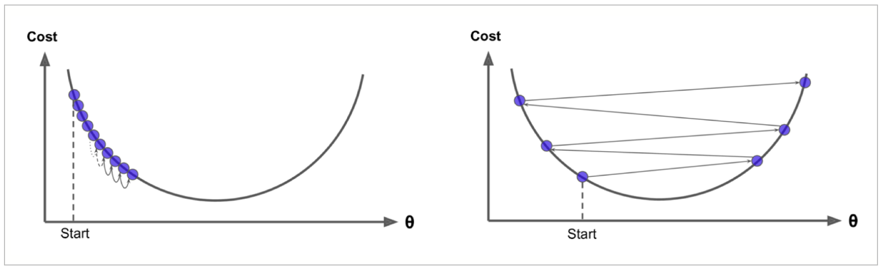
4.3 Linear Regression — Numerical Optimisation

To overcome these limitations, we consider a first order iterative numerical optimisation algorithm, **Gradient Descent**. Intuitively, we take steps proportional to the negative of the gradient (which is in the direction of steepest descent) at each step.

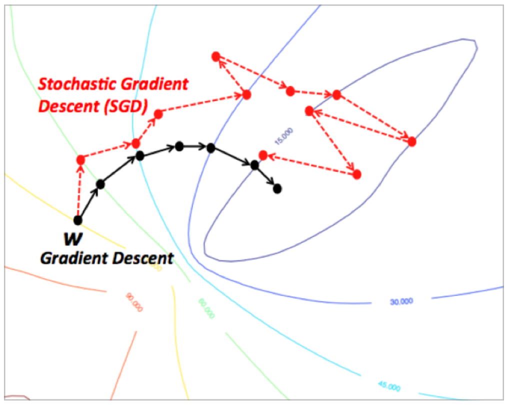
Batch Gradient Descent

```
def LinearRegression_OLS_GD(X, y, w_init, alpha, max_epoch=10):
    n = len(y)
    w_t = w_init
    L_hist = (1/(2*n)) * (y + np.matmul(X, w_t)).T.dot(y - np.matmul(X, w_t))
    w_hist = w_t.T
    epoch = 0
    while epoch < max_epoch:
        grad = (1/n) * X.T.dot(X.dot(w_t) - y).reshape(np.shape(X)[1], 1)
        w_t = (w_t - alpha * grad)
        loss = (1/(2*n)) * (y - X.dot(w_t)).T.dot(y - X.dot(w_t))[0][0]
        L_hist = np.vstack((L_hist, loss))
        w_hist = np.vstack((w_hist, w_t.T))
        epoch += 1
    return w_hist, L_hist
```

$\alpha > 0$ is the learning rate which determines the step size (factor of proportionality to the gradient).For α too small, convergence is slow, and for α too large, we get divergence.
Since the loss function is a convex objective, gradient descent guarantees the local optimum found is a global optimum. However, Batch Gradient Descent may be costly, as we need to scan through the entire training set for each step.



Stochastic Gradient Descent



In Stochastic Gradient Descent, we randomly shuffle the dataset for each step, and estimate the gradient using one observation. Hence, each SGD update is less optimal than a BGD update, and it will not converge monotonically, but overall convergence is generally faster.

Data Scaling

For multi-dimensional data, even if we make an optimal setting of the learning rate, **ill-conditioning** of the loss surface may result in a slow convergence. This is caused by the gradient of the largest attribute dominating the overall gradient. We may alleviate the effect through data scaling to scale our attributes. This ensures that all parameters are updated in similar proportions, leading to faster convergence.

4.4 Polynomial Regression

In Polynomial Regression we learn a mapping $\mathbf{f_W} : \mathbb{R}^m \mapsto \mathbb{R}$ between input attributes x and an output y drawn from a function class $\mathcal{F}.\mathbf{f_w}$ is characterised by a weight vector $\mathbf{w}$:

$$\mathbf{f_w} = w \cdot \hat{z}$$

for some vector $\hat{z}$ to encode the attributes (with higher degree polynomials and cross-terms).
The design matrix X grows with the dimensionality of the input data and the degree of the polynomial.

Example (Polynomial of second degree with **2** attributes)**.**

$$X = \begin{bmatrix} 1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

In general, the total number of terms (or multinomial coefficients) is $\binom{k+p-1}{p-1}$ for p attributes in the k-th degree polynomial.

4.5 Polynomial Regression — OLS

We can generate a solution via the normal equations with an analogue to the normal equations.

- **Representation**

$$\mathcal{F} = \{\mathbf{w} \cdot \mathbf{x}\}$$

- **Evaluation**

$$\frac{1}{2}\sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})}\right)^2$$

- **Optimisation**

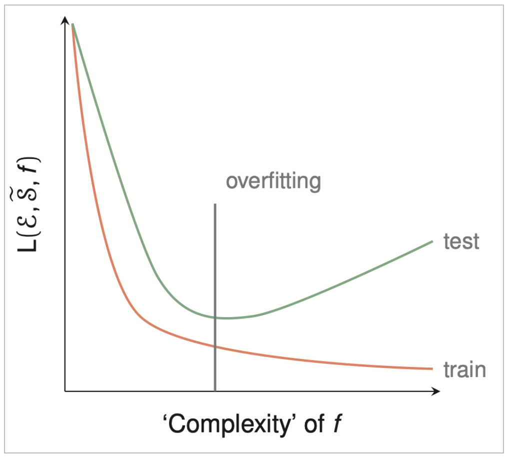
$$\mathbf{w}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \frac{1}{2}\sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})}\right)^2 \right\}$$

Overfitting vs. Underfitting

Underfitting occurs when we restrict ourselves to a representation that is not rich enough to encompass the relationships. This is characterised by high bias, and can be remedied by extending our representation to accommodate greater functional complexity.
While increasing functional complexity, we have the scope to overfit the data. This occurs when the model fits the residual variation (the noise) and contains more parameters that can be justified by the data. This results in poor generalisation. It can be characterised by high variance (between empirical and generalisation loss).

Learning Curves

To prevent underfitting and overfitting, we may compare how well the function performs on test data and training data:



Bias-Variance Tradeoff

We will never be able to completely reduce both effects in the absence of complete population data. As we increase the complexity of the function class the bias decreases but the variance increases as the hypothesis space grows.
The OLS analytical solution is given by the normal equations $\mathbf{w} = \mathbf{X^T X}^{-1}\mathbf{X^T y}$. For $X \in \mathbb{R}^{n\times k+1}$, $\mathbf{X^T X}$ is non-invertible if $k+1 > n$ and we do not have a unique solution.

Remark. With a high enough degree polynomial we can always reduce our training error to zero.

This can be remedied through regularisation, to manage model complexity. Intuitively, this reduces potential for larger magnitude weights related to higher complexity, and shrinks some of the weights towards zero.

Regularisation

In adoption of a Bayesian perspective, we model $\mathbf{w}$ as a random variable, and the MAP solution to weight optimisation results in a regularised objective. Depending on the distribution we select for $\mathbf{w}$, we may derive ridge regression or LASSO.
With the PAC approach, we model a worst case probabilistic bound on the generalised evaluation

function $E_{\mathcal{D}}[L]$ given some function class. We may also derive ridge regression or LASSO depending on which function class is selected.

4.6 Polynomial Regression — Ridge Regression

In Ridge Regression we optimise the empirical squared error loss function subject to a constraint on $\|\mathbf{w}\|_2 \leq t$.

- **Representation**

$$\mathcal{F} = \left\{ \mathbf{w} \cdot \mathbf{x} | \|\mathbf{w}\|_2^2 \leq t \right\}$$

- **Evaluation**

$$\frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})})^2$$

- **Optimisation**

$$\mathbf{w}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})})^2 + \frac{\lambda}{2} \sum_{i=1}^{m+1} \left(w^{(i)} \right)^2 \right\}$$

Using Lagrange Multipliers, our optimisation problem is now as follows:

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \lambda) = \mathbf{0}$$

$$\begin{aligned} \text{subject to:} \quad & \|\mathbf{w}\|_2^2 - t \leq 0 \\ & \lambda \geq 0 \\ & \lambda \left(\|\mathbf{w}\|_2^2 - t \right) = 0 \end{aligned}$$

where $\mathcal{L}(\mathbf{w}, \lambda) = \frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(i)^2} \right) + \frac{\lambda}{2} \left(\|\mathbf{w}\|_2^2 - t \right)$
If $\lambda = 0$, the constraint is redundant, and the solution is the non-regularised one. If $\lambda > 0$, $\|\mathbf{w}\|_2^2 = t$ and we have an equality constraint.
For any given t, we can find the optimal λ^* by solving for $\nabla_\lambda \mathcal{L}(\mathbf{w}, \lambda^*) = \mathbf{0}$. Additionally, $\mathcal{L}$ is convex w.r.t. $\mathbf{w}$ and we achieve optimum at $\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \lambda) = \mathbf{0}$. The new evaluation function then corresponds to this new objective:

$$\tilde{L}(\mathcal{E}, \mathcal{S}, \mathbf{f_w}) = \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

We can then solve for optimal $\mathbf{w}_{RR}$:

$$\begin{aligned} \nabla_{\mathbf{w}} \tilde{L} =& \mathbf{X^T X w} - \mathbf{X^T y} + \lambda \mathbf{w} \\ \mathbf{w}_{RR} =& \left(\mathbf{X^T X} + \lambda \mathbf{I} \right)^{-1} \mathbf{X^T y}. \end{aligned}$$

Since the Hessian $\mathcal{H} = \left(\mathbf{X^T X} + \lambda \mathbf{I} \right) \succeq 0$ and is always invertible, $\tilde{L}$ is strictly convex and we obtain an unique solution (with gradient descent).

Complexity Tuning

The regularisation parameter λ and polynomial degree k together are complexity tuning hyperparameters:

- High λ, low $k \implies$ low functional complexity $\implies$ underfitting
- Low λ, high $k \implies$ high functional complexity $\implies$ overfitting

However, in ridge regression, with a large number of weights, most of the regularised weights can shrink to almost zero but will rarely reach zero. This makes model interpretation difficult, especially with large number of parameters.

4.7 Polynomial Regression — LASSO

In LASSO, we optimise for the empirical squared error loss function, now subject to a contraint on $\|\mathbf{w}\|_1 \leq t$. This has the effect of shrinking some weights more aggressively to zero.

- **Representation**
$$\mathcal{F} = \{\mathbf{w} \cdot \mathbf{x} | \, \|\mathbf{w}\|_1 \leq t\}$$
- **Evaluation**
$$\frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})}\right)^2$$
- **Optimisation**
$$\mathbf{w}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})}\right)^2 + \frac{\lambda}{2} \sum_{i=1}^{m+1} \left(w^{(i)}\right) \right\}$$

However the evaluation function

$$\tilde{L}\left(\mathcal{E}, \mathcal{S}, \mathbf{f_w}\right) = \frac{1}{2} \sum_{i=1}^{n} \left(\mathbf{y} - \mathbf{X}\mathbf{w}\right)^T \left(\mathbf{y} - \mathbf{X}\mathbf{w}\right) + \frac{\lambda}{2} \|\mathbf{w}\|_1$$

is non-differentiable and we cannot look for stationary points in order to solve. We consider the subgradients:

$$\begin{cases} \frac{\partial L}{\partial w_j} + \frac{\lambda}{2} & \text{for } w_j > 0 \\ \frac{\partial L}{\partial w_j} - \frac{\lambda}{2} & \text{for } w_j < 0 \end{cases}$$

At $w_j = 0$ we are at an optimal point if

$$\frac{\partial L}{\partial w_j} + \frac{\lambda}{2} > 0 \quad \text{and;} \quad \frac{\partial L}{\partial w_j} - \frac{\lambda}{2} < 0$$
$$\implies \frac{\lambda}{2} < \frac{\partial L}{\partial w_j} < \frac{\lambda}{2}$$

Limitations

- When dealing with high dimensional data with few examples ($n < k + 1$), LASSO selects at most n variables before it saturates.
- With a highly correlated set of variables, LASSO tends to select one from the group and ignore the others.
- LASSO optimisation is not necessarily strictly convex, and in general will not yield an unique solution.

4.8 Polynomial Regression — Elastic Net

In Elastic Net Regularisation, Ridge Regression and LASSO is combined to remedy various shortcomings.

- **Representation**
$$\mathcal{F} = \left\{ \mathbf{w} \cdot \mathbf{x} | \|\mathbf{w}\|_2^2 \leq t_1 \wedge \|\mathbf{w}\|_1 \leq t_2 \right\}$$
- **Evaluation**
$$\frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})}\right)^2$$
- **Optimisation**
$$\mathbf{w}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})}\right)^2 + \frac{\lambda}{2} \left(\alpha \sum_{i=1}^{m+1} \left(w^{(i)}\right)^2 + (1-\alpha) \sum_{i=1}^{m+1} w^{(i)} \right) \right\}$$
for some $0 \leq \alpha \leq 1, \lambda \geq 0$

Beneficial Properties

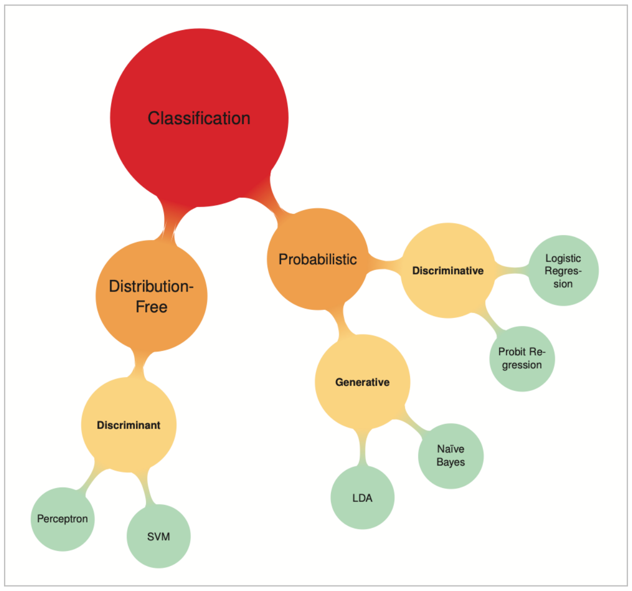
- Objective is strictly convex, and optimal Elastic Net weights are unique.
- The 1-norm term promotes sparsity.
- The 2-norm term promotes a grouping effect and removes the limitation on the number of selected variables.

5 Classification

In Classification we learn a mapping $f : \mathbb{R}^{m+1} \mapsto \{0, 1, \ldots, k\}$, drawn from a function class {.

- **Representation**
$$f \in \mathcal{F}$$
- **Evaluation**
$$\text{Loss Measure: } \mathcal{E}\left(f\left(\mathbf{x}\right), y\right) = \mathbb{I}\left[y \neq f(\mathbf{x})\right]$$
$$\text{Generalisation Loss: } L(\mathcal{E}, \mathcal{D}, f) = \mathbb{E}_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathcal{X})\right]\right]$$
- **Optimisation**
$$f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \left\{ \mathbb{E}_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathcal{X})\right]\right] \right\}$$

Classification Approaches



Distribution-free Classification paradigm: We seek to learn the classification boundary directly without probabilistic inference. e.g. PAC approach where we seek to approximate $\mathbb{E}_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathcal{X})\right]\right]$.
Probabilitistic Classification paradigm: The classification problem reduces to an inference problem in which we learn the posterior output class probability, each $p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right)$characterising an inhomogeneous Bernoulli distribution, for which we must parameterise a distribution for each $\mathbf{x} \in dom(\mathcal{X})$
Generative Classification: To learn $p_{\mathcal{Y}}(y|\mathbf{x})$ indirectly by inferring the likelihood $p_{\mathcal{X}}(\mathbf{x}|y)$ and the prior $p_{\mathcal{Y}}(y)$ for each class separately. Requires the most number of parameters to learn, but allows us to learn $p_{\mathcal{X}}(\mathbf{x})$.
Discriminative Classification: To learn $p_{\mathcal{Y}}(y|\mathbf{x})$ directly. Less demanding in terms of number of parameters to learn, but is inflexible, requiring re-running the lagorithm for changes of the loss function and does not deal well with class imbalances.

5.1 Baye's Optimal Classifier

For the binary classification problem, we have Baye's Optimal Classifier minimising misclassification loss:

$$f*(\mathbf{x}) = \begin{cases} 1 & \text{if} \quad p_{\mathcal{Y}}(y=1|\mathbf{x}) \geq 0.5 \\ 0 & \text{if} \quad p_{\mathcal{Y}}(y=1|\mathbf{x}) < 0.5 \end{cases}$$

Proof.

$$\begin{aligned}
f^* &= \underset{f\in\mathcal{F}}{\operatorname{argmin}} \left\{\mathbb{E}_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathcal{X})\right]\right]\right\} \\
&= \underset{f\in\mathcal{F}}{\operatorname{argmin}} \left\{ \sum_{y\in\{0,1\}} \int p_{\mathcal{Y}}(y|x)p_{\mathcal{X}}(\mathbf{x})\mathbb{I}\left[y \neq f(\mathbf{x})\right] \, d\mathbf{x} \right\} \\
&= \underset{f\in\mathcal{F}}{\operatorname{argmin}} \left\{ \sum_{y\in\{0,1\}} \int p_{\mathcal{Y}}(y|x)p_{\mathcal{X}}(\mathbf{x}) \left(f\left(\mathbf{x}\right)(1-y) + \left(1-f\left(\mathbf{x}\right)\right)y\right) \, d\mathbf{x} \right\} \\
&= \underset{f\in\mathcal{F}}{\operatorname{argmin}} \left\{ \int \left(p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right)\left(1-f\left(\mathbf{x}\right)\right) + p_{\mathcal{Y}}\left(y=0|\mathbf{x}\right) f\left(\mathbf{x}\right)\right) p_{\mathcal{X}}(\mathbf{x})\, d\mathbf{x} \right\} \\
&= \underset{f\in\mathcal{F}}{\operatorname{argmin}} \left\{ \int \left(p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right)\left(1-f\left(\mathbf{x}\right)\right) + \left(1-p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right)\right) f\left(\mathbf{x}\right)\right) p_{\mathcal{X}}(\mathbf{x})\, d\mathbf{x} \right\} \\
&= \underset{f\in\mathcal{F}}{\operatorname{argmin}} \left\{ \int \left(p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right) + f\left(\mathbf{x}\right)\left(1-2p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right)\right)\right) p_{\mathcal{X}}(\mathbf{x})\, d\mathbf{x} \right\}
\end{aligned}$$

Let $M(\mathbf{x}) = p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right) + f\left(\mathbf{x}\right)\left(1-2p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right)\right)$.
We need to find function f^* that is optimal for all $\mathbf{x} \in dom(\mathcal{X})$,

$$f^*(\mathbf{x}) = \underset{f(\mathbf{x})}{\operatorname{argmin}} \left\{M(\mathbf{x})\right\}$$

If $f^*(\mathbf{x}) = 1$ optimality implies:

$$1 - p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right) \leq p_{\mathcal{Y}}\left(y=1|x\right) p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right) \geq 0.5$$

■

Remark. WLOG, we may consider the Bayes Optimal Classifier for Generative Classification as follows:

$$\begin{aligned}
f^*(\mathbf{x}) &= \underset{y\in\{0,1\}}{\operatorname{argmax}} \left\{p_{\mathcal{Y}}(y|\mathbf{x})\right\} \\
&= \underset{y\in\{0,1\}}{\operatorname{argmax}} \left\{ \frac{p_{\mathcal{X}}\left(\mathbf{x}|y\right) P_{\mathcal{Y}}(y)}{\sum_{y\in\{0,1\}} p_{\mathcal{X}}(\mathbf{X}|y)p_{\mathcal{Y}}(y)} \right\} \\
&= \underset{y\in\{0,1\}}{\operatorname{argmax}} \left\{p_{\mathcal{X}}(\mathbf{x}|y)p_{\mathcal{Y}}(y)\right\}
\end{aligned}$$

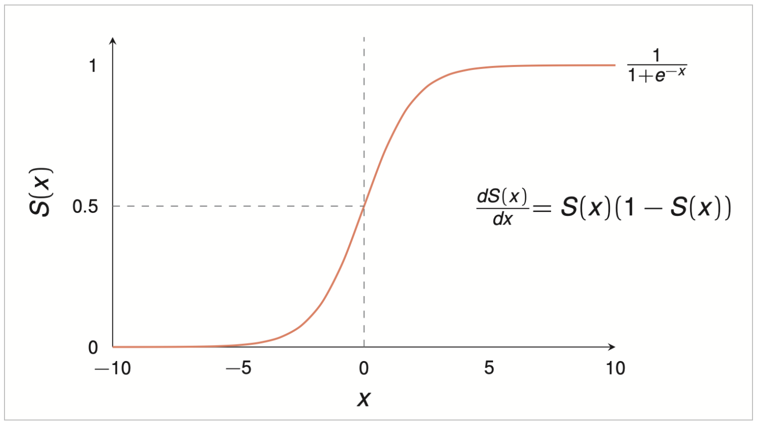
5.2 Logistic Regression

We seek to model $p_{\mathcal{Y}}(y=1|\mathbf{x})$ with a function $f : \mathbb{R}^m \mapsto [0,1]$. In Logistic Regression, we assume that the probability can be modelled by the logistic sigmoid:

$$S(x) = \frac{1}{1+e^{-\mathbf{w}\cdot\mathbf{x}}}.$$

- **Representation**

$$\mathcal{F} = \left\{ f_{\mathbf{w}}\left(\mathbf{x}\right) = \mathbb{I}\left[p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right) \geq 0.5\right] | p_{\mathcal{Y}}\left(y=1|\mathbf{x}\right) = \frac{1}{1+e^{-\mathbf{w}\cdot\mathbf{x}}}, \mathbf{w} \in \mathbb{R}^{m+1} \right\}$$



- **Evaluation**

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} y^{(i)}\mathbf{w}\cdot\mathbf{x}^{(\mathbf{i})} - \ln\left(1 + e^{\mathbf{w}\cdot\mathbf{x}^{(\mathbf{i})}}\right)$$

- **Optimisation**

$$\mathbf{w}_{MLE} = \underset{\mathbf{w}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ln\left(1 + e^{\mathbf{w}\cdot\mathbf{x}^{(i)}}\right) - y^{(i)}\mathbf{w}\cdot\mathbf{x}^{(i)}\right\}$$

Rearranging, we have

$$\begin{aligned}
p_{\mathcal{Y}}\left(y = 1|\mathbf{x}\right) =& \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{x}}}\\
e^{-\mathbf{w}\cdot\mathbf{x}} =& \frac{1}{p_{\mathcal{Y}}(y = 1|\mathbf{x})} - 1\\
\mathbf{w}\cdot\mathbf{x} =& \ln\left(\frac{p_{\mathcal{Y}}(y = 1|\mathbf{x})}{1 - p_{\mathcal{Y}}(y = 1|\mathbf{x})}\right)\\
=& logit(p_{\mathcal{Y}}(y = 1|\mathbf{x}))
\end{aligned}$$

Remark. $\mathbf{w}\cdot\mathbf{x} = 0$ defines a linear discriminant separating hyperplane.

Evaluation

With the logistic regression model, we have the following:

$$\mathcal{Y}\left(y = 1|\mathbf{x}\right) = \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{x}}}$$

$$\begin{aligned}
p_{\mathcal{Y}}\left(y = 0|\mathbf{x}\right) =& \frac{e^{-\mathbf{w}\cdot\mathbf{x}}}{1 + e^{-\mathbf{w}\cdot\mathbf{x}}}\\
=& \frac{1}{1 + e^{\mathbf{w}\cdot\mathbf{x}}}
\end{aligned}$$

We can then derive the Cross-Entropy loss function for logistic regression:

$$\begin{aligned}\mathcal{L}(\mathbf{w}) =& \ln\left(\prod_{i=1}^{n} p_{\mathcal{Y}}\left(y^{(i)}|\mathbf{x}^{(i)}\right)\right)\\ =& \sum_{i=1}^{n}\ln\left(p_{\mathcal{Y}}\left(y^{(i)}|\mathbf{x}^{(i)}\right)\right)\\ =& \sum_{i=1}^{n} y^{(i)}\ln\left(p_{\mathcal{Y}}\left(y^{(i)}=1|\mathbf{x}^{(i)}\right)\right)+\left(1-y^{(i)}\right)\ln\left(p_{\mathcal{Y}}\left(y^{(i)}=0|\mathbf{x}^{(i)}\right)\right)\\ =& \sum_{i=1}^{n}\ln\left(p_{\mathcal{Y}}\left(y^{(i)}=0|\mathbf{x}^{(i)}\right)\right)+y^{(i)}\ln\left(\frac{p_{\mathcal{Y}}\left(y^{(i)}=1|\mathbf{x}^{(i)}\right)}{p_{\mathcal{Y}}\left(y^{(i)}=0|\mathbf{x}^{(i)}\right)}\right)\\ =& \sum_{i=1}^{n} y^{(i)}\mathbf{w}\cdot\mathbf{x}^{(\mathbf{i})}-\ln\left(1+e^{\mathbf{w}\cdot\mathbf{x}^{(\mathbf{i})}}\right)\end{aligned}$$

Hence we seek $\mathbf{w}_{MLE}$:

$$\mathbf{w}_{MLE}=\underset{\mathbf{w}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n}\ln\left(1+e^{\mathbf{w}\cdot\mathbf{x}^{(i)}}\right)-y^{(i)}\mathbf{w}\cdot\mathbf{x}^{(i)}\right\}$$

Motivation

We assume some latent random variable $\mathcal{Y}^*$ such that $y^*=\mathbf{w}\cdot\mathbf{x}+\epsilon$ where $\epsilon\sim \mathit{Logistic}(0,1)$. Then

$$\varepsilon\sim \mathit{Logistic}(\mu,s)\quad\text{where:}\quad \mu\in\mathbb{R}, s>0.$$

Definition (Logistic Distribution)**.** The Logistic Distribution has the characteristic pdf:

$$f_\epsilon(\varepsilon;\mu,s)=\frac{e^{-\frac{\varepsilon-\mu}{s}}}{s\left(1+e^{-\frac{\varepsilon-\mu}{s}}\right)^2}.$$

$$E_{\mathcal{D}}[\epsilon]=\mu.$$

$$P(\epsilon<z)=\frac{1}{1+e^{-\frac{z-\mu}{s}}}.$$

We link a latent variable outcome to an output assuming the classification model:

$$y^{(i)}=\begin{cases}1 & \text{if} \quad y^{*(i)}\geq 0\\ 0 & \text{if} \quad y^{*(i)}<0\end{cases}.$$

$$\begin{aligned}p_{\mathcal{Y}}\left(y^{(i)}=1|\mathbf{x}^{(i)}\right)=& P\left(\mathcal{Y}^{*(i)}\geq 0|\mathbf{x}^{(i)}\right)\\ =& P\left(\mathbf{w}\cdot\mathbf{x}^{(i)}+\varepsilon^{(i)}\geq 0\right)\\ =& 1-\frac{1}{1+e^{\mathbf{w}\cdot\mathbf{x}^{(i)}}}\\ =& \frac{e^{\mathbf{w}\cdot\mathbf{x}^{(i)}}}{1+e^{\mathbf{w}\cdot\mathbf{x}^{(i)}}}\\ =& \frac{1}{1+e^{-\mathbf{w}\cdot\mathbf{x}^{(i)}}}\end{aligned}$$

Optimisation

However, the $\mathbf{w}_{MLE}$ we seek has no analytic solution. We may apply a numerical technique to optimise. This optimisation is a convex problem, hence the local optimum found would also be a global optimum.

$$\nabla^2_{\mathbf{w}}\mathcal{L} \geq 0.$$

Proof.

$$\begin{aligned}\nabla_{\mathbf{w}}(-y\mathbf{w}\cdot\mathbf{x}) &= -\,y\mathbf{x}\\ \nabla^2_{\mathbf{w}}(-y\mathbf{w}\cdot\mathbf{x}) &= \mathbf{0}\\ \implies \mathcal{H} &= \mathbf{0}\end{aligned}$$

$-y\mathbf{w}\cdot\mathbf{x}$ is convex.

$$\begin{aligned}\nabla_{\mathbf{w}}\left(\ln(1+e^{\mathbf{w}\cdot\mathbf{x}})\right) &= \frac{e^{\mathbf{w}\cdot\mathbf{x}}}{1+e^{\mathbf{w}\cdot\mathbf{x}}}\mathbf{x}\\ \frac{\partial \ln(1+e^{\mathbf{w}\cdot\mathbf{x}})}{\partial w_i} &= \frac{e^{\mathbf{w}\cdot\mathbf{x}}}{1+e^{\mathbf{w}\cdot\mathbf{x}}}x_i\\ \frac{\partial^2 \ln(1+e^{\mathbf{w}\cdot\mathbf{x}})}{\partial w_i \partial w_j} &= \frac{e^{\mathbf{w}\cdot\mathbf{x}}}{(1+e^{\mathbf{w}\cdot\mathbf{x}})^2}x_i x_j\\ \mathcal{H} &= \frac{e^{\mathbf{w}\cdot\mathbf{x}}}{(1+e^{\mathbf{w}\cdot\mathbf{x}})^2}\mathbf{x}\mathbf{x}^T\\ \implies \mathcal{H} &\succeq 0\end{aligned}$$

The objective is convex. ■

Linearly Separable Data

Consider that the training data is linearly separable. Consider the objective function for some $w = c\tilde{w}, c > 0$:

$$\sum_{i=1}^{n} \ln\left(1+e^{c\tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)}}\right) - y^{(i)}c\tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)}$$

Taking the derivative with respect to c, we have:

$$\sum_{i=1}^{n} \tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)}\left(\frac{e^{c\tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)}}}{1+e^{c\tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)}}} - y^{(i)}\right).$$

Since the data is well classified, there always exists a $\tilde{w}$ such that the objective has a negative derivative with respect to c, and gradient descent will cause c to grow without bound. The sigmoid function approaches a Heaviside function. This is a case of overfitting and can be circumvented through regularisation:

$$\sum_{i=1}^{n} \ln\left(1+e^{c\tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)}}\right) - y^{(i)}c\tilde{\mathbf{w}}\cdot\mathbf{x}^{(i)} + \lambda c^2 \left\|\tilde{\mathbf{w}}\right\|_2^2$$

We may discern a unique stationary point with respect to c with the derivative, using the addition of a Ridge Regulariser. Apart from the linearly separable non-regularised case, Logistic Regression in general leads to unique solutions.

Multinomial Logistic Regression

Supposing we have k classes such that $y \in \{1, \dots, k\}$, the Bayes Optimal Classifier becomes:

$$f^*(\mathbf{x}) = \underset{y\in\{1,\dots,k\}}{\text{argmax}} \{p_\mathcal{Y}(y|\mathbf{x})\}.$$

The model is now defined using the softmax function, and we seek to learn an inhomogeneous multinomial distribution:

$$p_\mathcal{Y}(y = k|\mathbf{x}) = \frac{e^{\mathbf{w}_j\cdot\mathbf{x}}}{\sum_{j=1}^{k} e^{\mathbf{w}_j\cdot\mathbf{x}}}.$$

The maximum likelihood solution will now make use of the multinomial cross entropy which results in a convex optimisation problem.

5.3 Naïve Bayes

In Naïve Bayes, we simplify the likelihood by assuming the conditional independence assumption of the input attributes given $\mathcal{Y}$:

$$p_\mathcal{X}(\mathbf{x}|y) = \prod_{i=1}^{m} p_{\mathcal{X}_\rangle}(x_i|y)$$

Supposing $\mathcal{Y}$ is a Bernoulli random variable, $y \sim Bern(\theta_y)$. We find the log-likelihood function:

$$\begin{aligned}\mathcal{L}(\theta) &= \ln\left(\prod_{i=1}^{n} p_\mathcal{Y}\left(y^{(i)};\theta_y\right)\right)\\ &= \sum_{i=1}^{n} \ln\left(p_\mathcal{Y}\left(y^{(i)};\theta_y\right)\right)\\ &= \sum_{i=1}^{n} y^{(i)}\ln\theta_y + \left(1-y^{(i)}\right)\ln(1-\theta_y)\end{aligned}$$

Hence we seek θ_{yMLE} such that:

$$\theta_{yMLE} = \underset{\theta_y}{\text{argmax}}\left\{\sum_{i=1}^{n} y^{(i)}\ln\theta_y + \left(1-y^{(i)}\right)\ln(1-\theta_y)\right\}$$

Taking the derivative and setting to 0, we have:

$$\begin{aligned}\nabla_{\theta_y} L &= \sum_{i=1}^{n}\frac{y^{(i)}}{\theta_y} - \frac{(1-y^{(i)})}{1-\theta_y}\\ \implies \theta_{yMLE} &= \frac{n_1}{n}\end{aligned}$$

Categorical Naïve Bayes

Suppose that the features x_i are discrete-valued and take m_i different values, such that each outcome x_i is taken from the set $\{x_{ij}\}_{j=1}^{m_i}$

- **Representation**

$$\mathcal{F} = \left\{ f_{\theta_y,\{\theta_{ijk}\}}(\mathbf{x}) = \underset{y\in\{0,1\}}{\text{argmax}}\left\{p_\mathcal{Y}(y)\prod_{i=1}^{m} p_{\mathcal{X}_\rangle}(x_i|y)\right\} \mid p_\mathcal{Y}(y=1) = \theta_y, \left\{p_{\mathcal{X}_\rangle}(x_{ij}|k) = \theta_{ijk}\right\}_{i=1,j=1,k=0}^{m,m_i,1}\right\}.$$

- **Evaluation**

$$\ln\left(L(\theta_y)\right) \quad \text{and} \quad \{\ln\left(L\left(\theta_{ik}\right)\right)\}_{i=1,k=0}^{m,1}$$

- **Optimisation**

$$\theta_{yMLE} = \frac{n_1}{n} \quad \text{and} \quad \left\{\theta_{ijkMLE} = \frac{n_{ijk}}{n_k}\right\}_{i=1,j=1,k=0}^{m,m_i,1}$$

Each $(x_i|y=k)$ is a categorical random variable, of which we seek to parameterise its categorical distribution.

Definition (Categorical Distribution)**.** The Categorical Distribution is a generalisation of the Bernoulli Distribution with more than 2 discrete outcomes (m_i discrete outcomes):

$$(\mathbf{x}_i|y=k) \sim Categorical(\Theta_{ik})$$

$$\Theta_{ik} \text{ has elements } \{\theta_{ijk}\}_{j=1}^{m_i}$$

$$p_{\mathcal{X}_\rangle}\left(\mathcal{X}_i = x_{ij}|y=k;\Theta_{ik}\right) = \theta_{ijk}$$

$$\sum_{j=1}^{m_i} \theta_{ijk} = 1$$

By forming the log-likelihood, and performing a constrained optimisation of the resulting function, we can obtain:

$$\theta_{ijkMLE} = \frac{n_{ijk}}{n_k}.$$

where n_{ijk} is the number of training points for which the i-th attribute belongs to the j-th category and $\mathcal{Y} = k$, and n_k is the number of training points of which $\mathcal{Y} = k$.

Additive Smoothing

To remedy the problem such that any category does not contain any instances, and prevent a case of overfitting where we estimate the probability of the event to be zero, we may utilise additive smoothing, adjusting the MLE estimates such that:

$$\theta_{ijk} = \frac{n_{ijk} + \alpha}{n_k + \alpha J}.$$

$$\theta_y = \frac{n_1 + \alpha}{n + \alpha K}.$$

where:

- $J = \#$ of distinct values outcomes of $\mathcal{X}_i$ can take (m_i in this case)
- $K = \#$ of distinct values outcomes of $\mathcal{Y}$ can take
- $\alpha =$ the strength of smoothing

Gaussian Naïve Bayes

Suppose that the features $x_i \in \mathbb{R}$ are continuous valued, such that each $(\mathcal{X}_i|y=k)$ is a Gaussian random variable, $(x_i|y=k) \sim \mathcal{N}(\mu_{ik}, \sigma_{ik})$. We then find the log-likelihood:

$$\begin{aligned}\mathcal{L}(\theta) &= \ln\left(\prod_{j=1}^{n_k} \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} \exp\left(-\frac{\left(x_i^{(j)}-\mu_{ik}\right)^2}{2\sigma_{ik}^2}\right)\right) \\ &= -n_k \ln \sigma_{ik} - \sum_{j=1}^{n_k}\left(-\frac{\left(x_i^{(j)}-\mu_{ik}\right)^2}{2\sigma_{ik}^2}\right) + const.\end{aligned}$$

We can optimise the log-likelihood with:

$$\mu_{ikMLE} = \sum_{j=1}^{n_k} \frac{x_i^{(j)}}{n_k}.$$

$$\sigma_{ikMLE}^2 = \frac{1}{n_k}\sum_{j=1}^{n_k}\left(x_i^{(j)}-\mu_{ik}\right)^2.$$

- **Representation**

$$\mathcal{F} = \left\{ f_{\theta_y,\{\theta_{ijk}\}}(\mathbf{x}) = \underset{y\in\{0,1\}}{\operatorname{argmax}} \left\{ py(y)\prod_{i=1}^{m}\mathcal{N}(X_i;\mu_{ik},\sigma_{ik})\right\} \mid py(y=1)=\theta_y, \{\mu_{ik}\in\mathbb{R}, \sigma_{ik}>0\}_{i=1,k=0}^{m,1}\right\}.$$

- **Evaluation**

$$\ln(L(\theta_y)) \quad \text{and} \quad \{\ln(L(\mu_{ik},\sigma_{ik}))\}_{i=1,k=0}^{m,1}$$

- **Optimisation**

$$\theta_{yMLE} = \frac{n_1}{n} \quad \text{and} \quad \left\{\mu_{ikMLE} = \sum_{j=1}^{n_k}\frac{x_i^{(j)}}{n_k}, \sigma_{ikMLE} = \frac{1}{n_k}\sum_{j=1}^{n_k}\left(x_i^{(j)}-\mu_{ik}\right)^2\right\}_{i=1,k=0}^{m,1}$$

Remark. GNB results in a similar form of linear discriminant as LR. However, they do not result in the same classifier, as GNB makes certain model assumptions that defines a dependence between w_0 and w_i.

5.4 Comparisons

Using a generative classifier requires learning more parameters than discriminative classifiers, but the generative approach is often intractable and require certain model assumptions (e.g. Conditional Independence). Since LR makes fewer model assumptions than a generative one such as NB, LR is considered more robust and less sensitive to modelling choices than NB, but NB requires less data for similar levels of convergence.

6 Model Selection

In Model Selection, we seek to choose the best hyperparameter / learning algorithm / model for a particular problem. We are primarily concerned with ranking a set of models, rather than estimating the performance of a particular model.

Measures for Performance

The measure of performance we are ultimately interested in is **Generalisation Loss**:

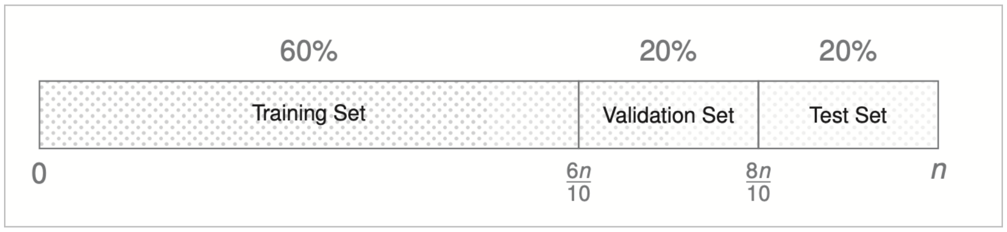
$$\mathbb{E}_{\mathcal{D}}\left[\mathcal{E}\left(f(\mathcal{X}), \mathcal{Y}\right)\right].$$

This cannot be directly measured, and empirical test set loss, $\mathbb{E}_{\mathcal{S}_{\mathcal{T}\rceil f \sqcup}}\left[\mathcal{E}\left(f(\mathcal{X}), \mathcal{Y}\right)\right]$ can act as a reasonable estimator (but not for model selection). Empirical Training Set Loss cannot be used as well, as it will lead to overfitting.
Hence, Empirical Risk Minimisation alone is not adequate to perform model selection.

6.1 Validation Techniques

We seek to estimate the generalisation loss through a **Validation Set Loss**. We split the training data into three sets:

- Training: To train each possible model
- Validation: To select the 'best' model
- Test: To assess the performance of that model



Validation Loss Bound

Applying the Hoeffding's Inequality to i.i.d. $\mathcal{Z}_i = \mathbb{I}\left[\mathcal{Y}^{(i)} \neq f\left(\mathbf{X}^{(i)}\right)\right]$:

$$P\left(E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \geq \frac{1}{n_v}\sum_{i=1}^{n_v} \mathbb{I}\left[y^{(i)} \neq f(\mathbf{x}^{(i)})\right] + \epsilon\right) \leq e^{-2n_v\epsilon^2}.$$

$$P\left(E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \geq E_{S_v}\left[\mathbb{I}\left[y^{(i)} \neq f(\mathbf{x}^{(i)})\right]\right] + \epsilon\right) \leq e^{-2n_v\epsilon^2}.$$

Let $\delta = e^{-2n_v\epsilon^2} \implies \epsilon = \sqrt{\frac{\ln\left(\frac{1}{\delta}\right)}{2n_v}}$.

$$P\left(E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] < E_{S_v}\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathbf{X})\right]\right] + \sqrt{\frac{\ln\left(\frac{1}{\delta}\right)}{2n_v}}\right) > (1-\delta).$$

That is, with probability greater than $(1-\delta)$, we state that:

$$L(\mathcal{E}, \mathcal{D}, f) \leq L(\mathcal{E}, \mathcal{S}_v, f) + \sqrt{\frac{\ln\left(\frac{1}{\delta}\right)}{2n_v}}.$$

Using the Union Bound, we can show that a bound holds for all members in a finite hypothesis class $\mathcal{F}$: Let A, B be the events:

$$A = \left\{ L(\mathcal{E}, \mathcal{D}, f^A) \leq L(\mathcal{E}, \mathcal{S}_v, f^A) + \sqrt{\frac{\ln\left(\frac{1}{\delta'}\right)}{2n_v}} \right\}.$$

$$B = \left\{ L(\mathcal{E}, \mathcal{D}, f^B) \leq L(\mathcal{E}, \mathcal{S}_v, f^B) + \sqrt{\frac{\ln\left(\frac{1}{\delta'}\right)}{2n_v}} \right\}.$$

We have $P(A) = P(B) < \delta'$.

Remark.

$$P(\neg A \wedge \neg B) \geq 1 - (P(A) + P(B)).$$

Combining these, $\forall f \in \{f^A, f^B\}$:

$$P\left(L(\mathcal{E}, \mathcal{D}, f) \leq L(\mathcal{E}, \mathcal{S}_v, f) + \sqrt{\frac{\ln\left(\frac{1}{\delta'}\right)}{2n_v}} \right) \geq 1 - 2\delta'.$$

Let $\delta = 2\delta'$, and we have:

$$P\left(L(\mathcal{E}, \mathcal{D}, f) \leq L(\mathcal{E}, \mathcal{S}_v, f) + \sqrt{\frac{\ln\left(\frac{2}{\delta}\right)}{2n_v}} \right) \geq 1 - \delta.$$

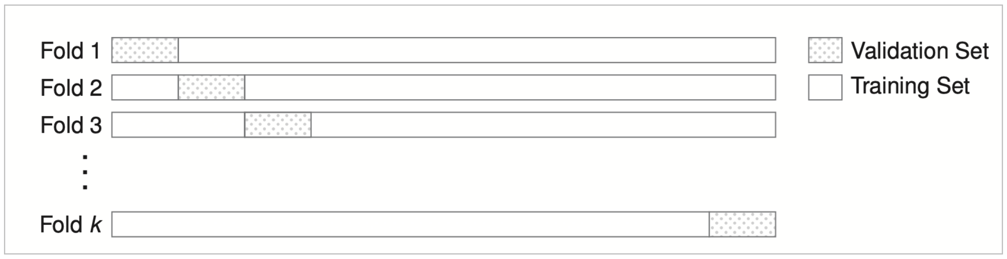
In general, $\forall f \in \mathcal{F}$:

$$P\left(L(\mathcal{E}, \mathcal{D}, f) \leq L(\mathcal{E}, \mathcal{S}_v, f) + \sqrt{\frac{\ln\left(\frac{|\mathcal{F}|}{\delta}\right)}{2n_v}} \right) \geq 1 - \delta.$$

The validation is a good estimate provided $\mathcal{F}$ is not too large, and n_v is not too small. Otherwise, the validation and generalisation losses will vary further as we begin to overfit.

6.2 Cross Validation

To retain most of our data for training, we perform validation while still maintaining the training data set, by spliting the training data into k folds. The learning algorithm is run k times for each model, each time using all the folds but one as the training set, and the remaining fold as the validation set. The cross validation loss is the performance averaged across all k folds:



$$L_{CV_k}(\mathcal{E}, \mathcal{S}, f) = \frac{1}{k} \sum_{i=1}^{k} L_{\mathcal{S} \backslash \mathcal{S}_k}(\mathcal{E}, \mathcal{S} \backslash \mathcal{S}_i, f).$$

k selection

$k = n$ is known as the Leave One Out cross validation, maximising the training set for each fold, is computation expensive, and fails to give a good estimate of the generalisation loss.
Empirical analysis suggests $k = 5$ or 10.

Limitations

There is not yet a rigorous understanding of why cross validation works well, and in certain circumstances should be treated with care.

Example (Time Series Data)**.** Requires sequential cross validation, due to similar neighbouring points.

6.3 PAC Approach

In the PAC (Probably Approximately Correct) approach, we formulate a probabilistic 'worst-case' bound using the empirical training loss and some complexity penalty (taking into account $|\mathcal{F}|$). We then perform based on the model that provides the tightest bound.

We obtain these bounds using the Uniform Convergence approach, by first seeking a finite sample concentration inequality independent of $\mathcal{D}$ to one function f, then applying it uniformly across all $f \in \mathcal{F}$ via Union Bound or other measure of functional complexity.

We consider a probability of success $(1 - \delta)$, an approximation loss target ϵ, and a data generating process $\mathcal{D}$.

Consistent Learner

For a consistent learning algorithm that only outputs hypotheses consistent with the training data ($E_{\mathcal{S}}\left[\mathcal{E}(f(\mathcal{X}), \mathcal{Y})\right] = 0$), for $0 < \epsilon < 1, 0 < \delta < 1$ and a particular $f \in \mathcal{F} \land E_{\mathcal{D}}\left[\mathcal{E}\left(f(\mathbf{X}), \mathcal{Y}\right)\right] > \epsilon$:

$$P(f \text{ is consistent with 1 training ex.}) < (1 - \epsilon) < e^{-\epsilon}.$$

$$P(f \text{ is consistent with } n \text{ training ex.}) < (1 - \epsilon)^n < e^{-\epsilon n}.$$

Applying the Union Bound $\forall f \in \mathcal{F}$, we obtain:

$$P\left(E_{\mathcal{D}}\left[\mathcal{E}\left(f(\mathbf{X}), \mathcal{Y}\right)\right] > \epsilon, \text{ for at least one } f \in \mathcal{F}\right) < |\mathcal{F}|\, e^{-\epsilon n}.$$

Theorem (PAC Bound: Finite $\boldsymbol{\mathcal{F}}$, Consistent Learner)**.** *For all $0 < \epsilon < 1$, $0 < \delta < 1$, all data generating distributions $\mathcal{D}$, with probability of at least $(1 - \delta)$:*

$$\forall f \in \mathcal{F} \quad E_{\mathcal{D}}\left[\mathcal{E}\left(f(\mathcal{X}), \mathcal{Y}\right)\right] \leq \frac{1}{n} \ln\left(\frac{|\mathcal{F}|}{\delta}\right).$$

Agnostic Learner

For a learning algorithm which is not restricted in the hypotheses: Applying the Hoeffding's Inequality to i.i.d. $\mathcal{Z}_i = \mathbb{I}\left[\mathcal{Y}^{(i)} \neq f\left(\mathbf{X}^{(i)}\right)\right]$:

$$P\left(E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \geq \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}\left[y^{(i)} \neq f(\mathbf{x}^{(i)})\right] + \epsilon\right) \leq e^{-2n\epsilon^2}.$$

$$P\left(E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \geq E_S\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathbf{X})\right]\right] + \epsilon\right) > e^{-2n\epsilon^2}.$$

Similarly, we applying the Union Bound to obtain:

$$P\left(E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \geq E_S\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathbf{X})\right]\right] + \epsilon, \text{ for at least one } f \in \mathcal{F}\right) \leq \left|\mathcal{F}\right| e^{-2n\epsilon^2}.$$

Theorem (PAC Bound: Finite $\boldsymbol{\mathcal{F}}$, Agnostic Learner)**.** *For all* $0 < \epsilon < 1$*,* $0 < \delta < 1$*, all data generating distributions* $\mathcal{D}$*, with probability of at least* $(1 - \delta)$*:*

$$\forall f \in \mathcal{F} \quad E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \leq E_S\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathbf{X})\right]\right] + \sqrt{\frac{1}{2n}\ln\left(\frac{|\mathcal{F}|}{\delta}\right)}$$

Infinite $\mathcal{F}$

Theorem (PAC Bound: Infinite $\boldsymbol{\mathcal{F}}$, Agnostic Learner)**.** *For all* $0 < \epsilon < 1$*,* $0 < \delta < 1$*, all data generating distributions* $\mathcal{D}$*, with probability of at least* $(1 - \delta)$*:*

$$\forall f \in \mathcal{F} \quad E_{\mathcal{D}}\left[\mathbb{I}\left[\mathcal{Y} \neq f\left(\mathbf{X}\right)\right]\right] \leq E_S\left[\mathbb{I}\left[\mathcal{Y} \neq f(\mathbf{X})\right]\right] + 2\mathbb{R}\left(\mathcal{F} \circ \mathcal{S}\right) + 4\sqrt{\frac{2}{n}\ln\left(\frac{4}{\delta}\right)}$$

where $\mathbb{R}\left(\mathcal{F} \circ \mathcal{S}\right)$ *denotes the Rademacher complexity of* $\mathcal{F} \circ \mathcal{S} = \left\{f(\mathbf{x}^{(i)}) | f \in \mathcal{F}\right\}_{i=1}^{n}$

Advantages and Limitations

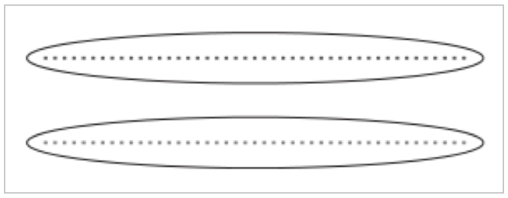
The PAC approach is not limited to misclassification loss, but to a variety of other loss functions. It allows comparison with training data alone while avoiding overfitting.

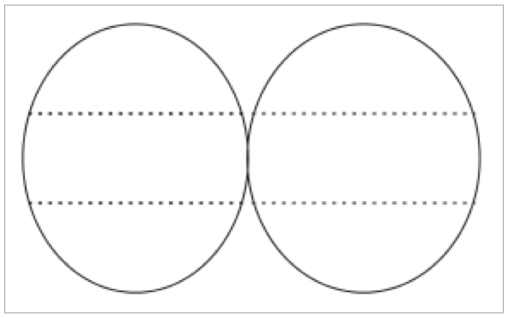
However, the bounds are often loose, and are poor estimators of generalisation loss, and tend to underperform cross validation.

7 Clustering

In Clustering, we seek to learn groups or clusters from our input data, and in so doing assign each instance to a cluster. Intuitively, we group objects such that similar objects end up in the same group.

Measures of Similarity





As measures of similarity, we can consider transitivity, where points are clustered according to whether they are closely related to neighbours regardless of how far apart the first and last neighbours are.
Alternatively, we may consider proximity, where points are clustered according to some mutual shared distance, of which they cluster around a shared point.

Evaluation

Without labels of our data, we often are unable to evaluate how well our predictions compare with the ground truth, and we are unsure of the number of "clusters".
It is hence not possible to have a clustering function that fits all kinds of data, but for different problem settings we may be able to employ different clustering algorithms:

- **Partitional Algorithms**: Algorithms such as k-means clustering, Spectral Clustering techniques that divide data into a fixed number of clusters directly
- **Hierachical Algorithms**: Algorithms that build a hierarchy of clusters by either merging or splitting, such as Agglomerative Clustering techniques

These clustering algorithms allow us to focus on specific tasks at hand, such as data exploration and data preprocessing.

7.1 k-means Algorithm

In k-means algorithm, instances that lie inside a cluster have small inter-point distances (similarity by proximity). Assuming we are interested in finding k clusters, of which the i-th cluster is represented by a centroid or prototype denoted $\mu^{[j]} \in \mathbb{R}^m$. We seek to find centroids such that the sum of squares of distances to each instance to its closest centroid is minimised.

Problem Setting

We have input data consisting of n-instances $\left\{\mathbf{x}^{(i)}\right\}_{i=1}^{n}$ where $\mathbf{x}^{(i)} \in \mathbb{R}^m$. For each instance, we create a set of indicator variables $\left\{\rho^{i[j]}\right\}_{j=1}^{k}$ where $\rho^{i[j]} \in \{0,1\}$ for whether $\mathbf{x}^{(i)}$ is assigned to cluster j. For each point $\mathbf{x}^{(i)}$, let:

$$j^* = \underset{l}{\operatorname{argmin}} \left\|\mathbf{x}^{(i)} - \mu^{[l]}\right\|_2^2 .$$

$$\rho^{i[j]} = \begin{cases} 1, & \text{if } j = j^* \\ 0 & \text{otherwise} \end{cases} .$$

Our objective function is defined as the sum of squared distances between each instance and its assigned cluster:

$$\Theta = \sum_{i=1}^{n} \sum_{j=1}^{k} \rho^{i[j]} \left\|\mathbf{x}^{(i)} - \mu^{[j]}\right\|_2^2 .$$

This is known as the distortion function.

Optimisation

This function is hard to minimise: with ideal prototypes, we can solve by assigning data points to the nearest cluster; with ideal assignments, we could solve for the prototypes. The k-means algorithm, or **Lloyd's Algorithm** is a greedy algorithm that attempts to solve the optimisation problem:

- Start by choosing a initial (random) value for each $\mu^{[j]}$
- **E-Step**: Minimise Θ w.r.t. $\left\{\rho^{i[j]}\right\}_{i=1,j=1}^{n,k}$, keeping all $\mu^{[j]}$ constant.
  - Each of the n terms are independent and we can optimise each independently.
  - We choose $p^{i[j]} = 1$ for the value of j giving the minimum value of the squared Euclidean distances:
  $$\rho^{i[j]} = \begin{cases} 1, & \text{if } j = \text{argmin}_l \left\|\mathbf{x}^{(i)} - \mu^{[l]}\right\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$
- **M-Step**: Minimise Θ w.r.t. $\left\{\mu^{[j]}\right\}_{j=1}^{k}$, keeping all $\rho^{[j]}$ constant.
  - Θ is a convex quadratic function of $\mu^{[j]}$. Taking the derivative and setting it to zero, we obtain:
  $$2\sum_{i=1}^{n} \rho^{i[j]} \left(\mathbf{x}^{(i)} - \mu^{[j]}\right).$$
  $$\mu^{[j]} = \frac{\sum_{i=1}^{n} \rho^{i[j]}\mathbf{x}^{(i)}}{\sum_{i=1}^{n} \rho^{i[j]}}.$$
- The E-Step and M-Step are repeated until convergence.
  Proof. By definition,
  $$\Theta\left(\rho_{(t)}^{i[j]}, \mu_{(t)}^{[j]}\right) = \sum_{i=1}^{n}\sum_{j=1}^{k} \rho_{(t)}^{i[j]} \left\|\mathbf{x}^{(i)} - \mu_{(t)}^{[j]}\right\|_2^2.$$
  On the M-step:
  $$\Theta\left(\rho_{(t)}^{i[j]}, \mu_{(t)}^{[j]}\right) \leq \sum_{i=1}^{n}\sum_{j=1}^{k} \rho_{(t)}^{i[j]} \left\|\mathbf{x}^{(i)} - \mu_{(t-1)}^{[j]}\right\|_2^2.$$
  On the E-step:
  $$\sum_{i=1}^{n}\sum_{j=1}^{k} \rho_{(t)}^{i[j]} \left\|\mathbf{x}^{(i)} - \mu_{(t-1)}^{[j]}\right\|_2^2 \leq \sum_{i=1}^{n}\sum_{j=1}^{k} \rho_{(t-1)}^{i[j]} \left\|\mathbf{x}^{(i)} - \mu_{(t-1)}^{[j]}\right\|_2^2 = \Theta\left(\rho_{(t-1)}^{i[j]}, \mu_{(t-1)}^{[j]}\right).$$
  $$\therefore \Theta\left(\rho_{(t)}^{i[j]}, \mu_{(t)}^{[j]}\right) \leq \Theta\left(\rho_{(t-1)}^{i[j]}, \mu_{(t-1)}^{[j]}\right) \quad \blacksquare$$
  Hence the algorithm converges, but not necessarily to the global optimum.

Limitations

- k has to be specified prior to performing the algorithm.
- The object is non-convex, and the converged optimum is not necessarily global.
- Assumes clusters are hyperspheres, and works poorly on non-convex shaped clusters.
- Works poorly on clusters of different sizes.
- Sensitive to data-scaling
- Sensitive to noise and other small perturbations of data, due to hard assignments to clusters.

7.2 Gaussian Mixture Model

Latent Variable Models

Definition (Latent Variables)**.** Variables that cannot be observed directly, and can only be inferred through a model.

Definition (Latent Variable Model)**.** A statistical model that relates a set of observable variables to a set of latent variables.

Through usage of latent variable models, we are able to express joint distributions more efficiently at the expense of model assumptions. We assume conditional independence of the attributes on the latent variable.

Mixture Models

Not all random variables can be modelled solely with standard probability distribution functions. With a mixture model, we have access to a richer set of probability distribution functions (often multimodal).

Problem Setting

Consider a set of unlabelled points $\left\{\mathbf{x}^{(i)} \in \mathbb{R}^m\right\}_{i=1}^{n}$ and k clusters. Each point has an unknown latent cluster assignment associated with it, $z^{(i)} \in \{1, \ldots, k\}$, which is the outcome of a multinomial random variable $\mathcal{Z}$:

$$z^{(i)} \sim \text{Multinomial}\left(\pi^{[1], \ldots, \pi^{[k]}}\right).$$

$$p_{\mathcal{Z}}\left(z^{(i)} = j\right) = \pi^{[j]}, \quad \sum_{i=1}^{k} \pi^{[i]} = 1, \quad \pi^{[j]} \geq 0, \quad \forall j.$$

Additionally, each $\mathbf{x}^{(i)}$ is the outcome of a Gaussian random variable, $\mathcal{X}$:

$$\mathbf{x}^{(i)} | \left(z^{(i)} = j\right) \sim \mathcal{N}\left(\mathbf{x}^{(i)}; \mu^{[j]}, \mathbf{\Sigma}^{[j]}\right).$$

where $\mu^{[j]} \in \mathbb{R}^m, \mathbf{\Sigma}^{[j]} \in \mathbb{R}^{m \times m}$ are the mean and covariance associated with cluster j.
The joint distribution is hence given by:

$$p_{\mathcal{X},\mathcal{Z}}\left(\mathbf{x}^{(i)}, z^{(i)}\right) = p_{\mathcal{X}}\left(\mathbf{x}^{(i)} | z^{(i)}\right) p_{\mathcal{Z}}\left(z^{(i)}\right).$$

$$\begin{aligned} p_{\mathcal{X}}\left(\mathbf{x}^{(i)}\right) &= \sum_{z=1}^{k} p_{\mathcal{X}}\left(\mathbf{x}^{(i)}|z^{(i)}\right) p_{\mathcal{Z}}\left(z^{(i)}\right) \\ &= \sum_{j=1}^{k} \mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)\pi^{[j]} \end{aligned}$$

The unconditional probability of each $\mathbf{x}^{(i)}$ is modelled as a Gaussian Mixture Model.

Optimisation

We derive the log-likelihood:

$$\mathcal{L} = \sum_{i=1}^{n} \log\left(\pi^{[j]}\sum_{j=1}^{k}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)\right)$$

subject to:

$$\sum_{j=1}^{k}\pi^{[j]} = 1, \quad \mathbf{\Sigma}^{[j]} \succ 0$$

which is a constrained, non-concave optimisation problem. Differentiating L with respect to each variable, we have:

$$\begin{aligned} \nabla_{\mu^{[j]}} L &= \sum_{i=1}^{n} \frac{\partial L}{\partial \mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)} \frac{\partial \mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)}{\partial \mu^{[j]}} \\ &= \sum_{i=1}^{n} \frac{\pi^{[j]}}{\sum_{j=1}^{k}\pi^{[j]}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)} \frac{\partial \mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)}{\partial \mu^{[j]}} \\ &= \sum_{i=1}^{n} \frac{\pi^{[j]}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)}{\sum_{j=1}^{k}\pi^{[j]}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)} \frac{\partial}{\partial \mu^{[j]}} \log \mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right) \\ &= -\sum_{i=1}^{n}\gamma^{i[j]}\frac{1}{2}\frac{\partial}{\partial\mu^{[j]}}\left(\mathbf{x}^{(i)}-\mu^{[j]}\right)^{T}\mathbf{\Sigma}^{-1}\left(\mathbf{x}^{(i)}-\mu^{[j]}\right) \times \text{const.} \\ &= \sum_{i=1}^{n}\gamma^{i[j]}\mathbf{\Sigma}^{-1}\left(\mathbf{x}^{(i)}-\mu^{[j]}\right) \times \text{const.} \end{aligned}$$

where $\gamma^{i[j]} = \frac{\pi^{[j]}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)}{\sum_{j=1}^{k}\pi^{[j]}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)}$

$$\frac{\partial L}{\partial \Sigma^{[j]}} = \sum_{i=1}^{n}\gamma^{i[j]}\frac{\partial}{\partial \mathbf{\Sigma}^{[j]}}\log\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right).$$

Using Lagrange Multipliers to enforce the $\sum_{j=1}^{k}\pi^{[k]} = 1$ constraint, we have:

$$\mathcal{L} = \sum_{i=1}^{n}\log\left(\sum_{j=1}^{k}\pi^{[j]}\mathcal{N}\left(\mathbf{x}^{(i)};\mu^{[j]},\mathbf{\Sigma}^{[j]}\right)\right) + \lambda\left(\sum_{k=1}^{k}\pi_j - 1\right).$$

$$\frac{\partial \mathcal{L}}{\partial \pi^{[j]}} = \sum_{i=1}^{n} \frac{\gamma^{i[j]}}{\pi^{[j]}} + \lambda.$$

Solving for critical points of L with respect to each variable, we have:

$$\mu^{[j]*} = \frac{\sum_{i=1}^{n} \gamma^{i[j]} \mathbf{x}^{(i)}}{\sum_{i=1}^{n} \gamma^{i[j]}}.$$

$$\mathbf{\Sigma}^{[j]*} = \frac{\sum_{i=1}^{n} \gamma^{i[j]} \left(\mathbf{x}^{(i)} - \mu^{[j]}\right)\left(\mathbf{x}^{(i)} - \mu^{[j]}\right)^T}{\sum_{i=1}^{n} \gamma^{i[j]}}.$$

$$\pi^{[j]*} = \frac{1}{n} \sum_{i=1}^{n} \gamma^{i[j]}.$$

Responsibility

$\gamma^{i[j]}$ can be viewed as the responsibility that component j takes for explaining $\mathbf{x}^{(i)}$:

$$\gamma^{i[j]} = \frac{\pi^{[j]} \mathcal{N}\left(\mathbf{x}^{(i)}; \mu^{[j]}, \mathbf{\Sigma}^{[j]}\right)}{\sum_{j=1}^{k} \pi^{[j]} \mathcal{N}\left(\mathbf{x}^{(i)}; \mu^{[j]}, \mathbf{\Sigma}^{[j]}\right)}$$

Each optimal variable expression is in terms of the responsibility, and the responsibility itself is a function of the optimal variables.

Expectation Maximisation

Hence, we adopt an analoguue to the k-means algorithm to solve this problem.

- Start by choosing a initial (random) value for $\left\{\mu^{[j]*}, \mathbf{\Sigma}^{[j]*}, \pi^{[j]*}\right\}_{j=1}^{k}$
- **E-Step**: Compute the responsibilities $\gamma^{i[j]}$ given the current parameters
- **M-Step**: Minimise $\mathcal{L}$ w.r.t. $\left\{\mu^{[j]*}, \mathbf{\Sigma}^{[j]*}, \pi^{[j]*}\right\}_{j=1}^{k}$, keeping all $\gamma^{i[j]}$ constant.

$$\mu^{[j]*} = \frac{\sum_{i=1}^{n} \gamma^{i[j]} \mathbf{x}^{(i)}}{\sum_{i=1}^{n} \gamma^{i[j]}} \qquad \mathbf{\Sigma}^{[j]*} = \frac{\sum_{i=1}^{n} \gamma^{i[j]} \left(\mathbf{x}^{(i)} - \mu^{[j]}\right)\left(\mathbf{x}^{(i)} - \mu^{[j]}\right)^T}{\sum_{i=1}^{n} \gamma^{i[j]}} \qquad \pi^{[j]*} = \frac{1}{n} \sum_{i=1}^{n} \gamma^{i[j]}.$$

- The E-Step and M-Step are repeated until convergence.
  Proof. At the end of the t-th epoch, we have (By Jensen's Inequality):

$$\mathcal{L}\left(\theta_{(t)}\right) \leq \sum_{i} \sum_{z^{(i)}} q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right) \log\left(\frac{p_{\mathcal{X},\mathcal{Z}}\left(\mathbf{x}^{(i)}, z^{(i)}; \theta_{(t)}\right)}{q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right)}\right)$$

  In the preceding M-step,

$$\theta_{(t)} = \operatorname*{argmax}_{\theta} \left(q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right) \log\left(\frac{p_{\mathcal{X},\mathcal{Z}}\left(\mathbf{x}^{(i)}, z^{(i)}; \theta_{(t)}\right)}{q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right)}\right)\right).$$

$$\sum_i \sum_{z^{(i)}} q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right) \log\left(\frac{p_{\mathcal{X},\mathcal{Z}}\left(\mathbf{x}^{(i)}, z^{(i)}; \theta_{(t)}\right)}{q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right)}\right) \geq \sum_i \sum_{z^{(i)}} q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right) \log\left(\frac{p_{\mathcal{X},\mathcal{Z}}\left(\mathbf{x}^{(i)}, z^{(i)}; \theta_{(t-1)}\right)}{q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right)}\right)$$

RHS is the output of the preceding E-step, in which the tightest bound is achieved from setting $q_{\mathcal{Z}(t)}$:

$$\sum_i \sum_{z^{(i)}} q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right) \log\left(\frac{p_{\mathcal{X},\mathcal{Z}}\left(\mathbf{x}^{(i)}, z^{(i)}; \theta_{(t-1)}\right)}{q^{(i)}_{\mathcal{Z}(t)}\left(z^{(i)}\right)}\right).$$

$$\mathcal{L}\left(\theta_{(t)}\right) \geq \mathcal{L}\left(\theta_{(t-1)}\right) \quad \blacksquare$$

Similarly, the algorithm converges but not necessarily to the global optimum.

Relationship with k-means

Consider a GMM where we have 'spherical' clusters, i.e. $\mathbf{\Sigma}^{[j]} = \epsilon\mathbf{I}, \forall j, \epsilon =$const.:

$$p_{\mathcal{X}}\left(\mathbf{x}^{(i)} | z^{(i)} = j\right) = \frac{1}{(2\pi\epsilon)^{\frac{m}{2}}} \exp\left(-\frac{1}{2\epsilon}\left\|\mathbf{x}^{(i)} - \mu^{[j]}\right\|_2^2\right).$$

The responsibilities are given by:

$$\gamma^{i[j]} = \frac{\pi^{[j]} \exp\left(\frac{1}{2\epsilon}\left\|\mathbf{x}^{(i)} - \mu^{[j]}\right\|_2^2\right)}{\sum_j \pi^{[j]} \exp\left(\frac{1}{2\epsilon}\left\|\mathbf{x}^{(i)} - \mu^{[j]}\right\|_2^2\right)}$$

As $\epsilon \to 0$:

$$\gamma^{i[j]} \to \begin{cases} 1, & \text{if } j = \text{argmin}_g \left\|\mathbf{x}^{(i)} - \mu^{[g]}\right\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$
$$= \rho^{i[j]}$$

In this case, $pi^{[j]}$ no longer plays an active role and the only important M-step update is $\mu^{[j]}$. i.e. as $\epsilon \to 0$, GMM clustering $\to$ k-means.

Limitations

With GMM, we are able to accommodate for less restrictive cluster shapes and sizes than k-means (ellipsoids rather than circles). k can be selected with reference to validation set likelihood and is more robust than k-means.
The objective is non-convex and works poorly on non-convex clusters.

8 Dimensionality Reduction

In Dimensionality Reduction, we assume that although the data is high-dimensional, it lies on or near a low-dimensional subspace or manifold.

8.1 Principal Component Analysis

Considering a linear subspace $\mathbb{R}^d$ within $\mathbb{R}^m$ where $d << m$, we can reduce the dimensionality of our data, since we only require $\mathbb{R}^d$ coordinates to describe the point. For this problem, we consider Principal Component Analysis, a method of linear dimensionality reduction.

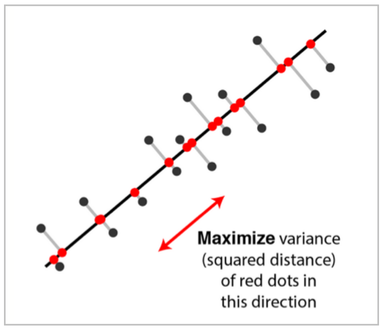
Problem Setting

We assume our data consists n instances: $\{\mathbf{x}^{(i)}\}_{i=1}^{n}$ where $\mathbf{x}^{(i)} \in \mathbb{R}^m$ of which we are projecting (lienarly) onto a space $\mathbb{R}^d$ where $d < m$ such that the variance of projected data is maximised. The space is spanned by a set of orthonormal basis vectors $\{\mathbf{u}^{[i]}\}_{i=1}^{d}$ where $\mathbf{u}^{[i]} \in \mathbb{R}^m$.
Additionaly, we define the mean of the projected data onto each basis vector $\mathbf{u}^{[j]} \cdot \overline{\mathbf{x}}$ where $\overline{\mathbf{x}}$ is the sample mean:

$$\overline{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}^{(i)}.$$

Projected Variance Maximisation

We adopt the view of PCA of Projected Variance Maximisation, where the idea is to project our high-dimensional data onto a lower-dimensional subspace such that sample variance is maximally preserved.



Definition (Sample Variance)**.** The sample variance of the projected data is given by:

$$\frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{u}^{[j]} \cdot \mathbf{x}^{(i)} - \mathbf{u}^{[j]} \cdot \overline{\mathbf{x}}\right)^2 = \mathbf{u}^{[j]T}\mathbf{S}\mathbf{u}^{[j]}$$

The sample covariance matrix $\mathbf{S}$ is defned by:

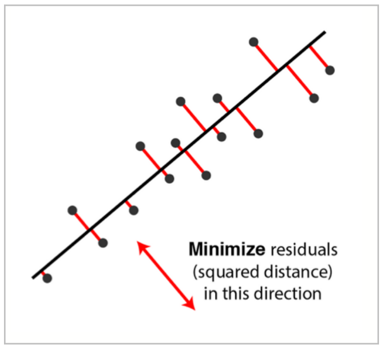
$$\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{x}^{(i)} - \overline{\mathbf{x}}\right)\left(\mathbf{x}^{(i)} - \overline{\mathbf{x}}\right)^T = \frac{1}{n}\mathbf{X}^T\mathbf{X}$$

where the centred design matrix $\mathbf{X}$ is defined:

$$\mathbf{X} = \begin{bmatrix} \left(\mathbf{x}^{(1)} - \overline{\mathbf{x}}\right)^T \\ \left(\mathbf{x}^{(2)} - \overline{\mathbf{x}}\right)^T \\ \vdots \\ \left(\mathbf{x}^{(n)} - \overline{\mathbf{x}}\right)^T \end{bmatrix}.$$

Remark. PCA can also be viewed as a search for the d-dimensional subspace minmising the reconstruction error:

$$\sum_{i=1}^{n}\left\|\left(\mathbf{x}^{(i)}-\overline{\mathbf{x}}\right)-\sum_{j=1}^{d}\left(\mathbf{u}^{[j]}\cdot\left(\mathbf{x}^{(i)}-\overline{\mathbf{x}}\right)\right)\mathbf{u}^{[j]}\right\|_2^2 .$$



Optimisation

Re-writing our optimisation problem, we have:

$$\underset{\{\mathbf{u}^{[j]}\}_{j=1}^{d}}{\operatorname{argmax}} L \quad \text{where:} \quad L=\sum_{j=1}^{d}\mathbf{u}^{[j]T}\mathbf{S}\mathbf{u}^{[j]}.$$

for some orthonormal $\{\mathbf{u}^{[i]}\}_{i=1}^{d}$.
In this algorithm, we attempt to learn each dimension greedily. We first search for the direction of highest variance, and write the objective as follows:

$$\mathcal{L}(\mathbf{u}^{[1]},\lambda^{[1]})=\mathbf{u}^{[1]T}\mathbf{S}\mathbf{u}^{[1]}-\lambda^{[1]}\left(\mathbf{u}^{[1]}\cdot\mathbf{u}^{[1]}-1\right)$$

for some lagrange multiplier $\lambda^{[1]}$ associated with the orthogonality constraint. Seeking stationarity w.r.t. $\mathbf{u}^{[1]}$, we have:

$$\begin{aligned}2\mathbf{S}\mathbf{u}^{[1]}-2\lambda^{[1]}\mathbf{u}^{[1]}=&0\\ \implies \mathbf{S}\mathbf{u}^{[1]}=&\lambda^{[1]}\mathbf{u}^{[1]}\end{aligned}$$

Hence $\mathbf{u}^{[1]}$ is an eigenvector of $\mathbf{S}$ associated with the eigenvalue $\lambda^{[1]}$. To find the variance of the projected data, we have:

$$\mathbf{u}^{[1]T}\mathbf{S}\mathbf{u}^{[1]}=\lambda^{[1]}$$

To maximise this variance, we select the eigenvector associated with the largest eigenvalue. We have found the first basis vector of greatest variance. Now we seek to the second basis vector $\mathbf{u}^{[2]}$ to further increase the projected variance, such that $\mathbf{u}^{[2]}\cdot\mathbf{u}^{[2]}=1$ and $\mathbf{u}^{[1]}\cdot\mathbf{u}^{[2]}=0$. We write the objective as follows:

$$\mathcal{L}(\mathbf{u}^{[2]},\lambda^{[2]},\lambda^{[1][2]|})=\mathbf{u}^{[2]T}\mathbf{S}\mathbf{u}^{[2]}-\lambda^{[2]}\left(\mathbf{u}^{[2]}\cdot\mathbf{u}^{[2]}-1\right)-\lambda^{[1][2]}\left(\mathbf{u}^{[2]}\cdot\mathbf{u}^{[1]}-0\right)$$

for some lagrange multipliers $\lambda^{[2]}, \lambda^{[1][2]}$. Seeking stationarity w.r.t. $\mathbf{u}^{[2]}$, we have:

$$2\mathbf{S}\mathbf{u}^{[2]} - 2\lambda^{[2]}\mathbf{u}^{[2]} - \lambda^{[1][2]}\mathbf{u}^{[1]} = 0.$$

Left multiplying with $\mathbf{u}^{[1]T}$, $\lambda^{[1][2]} = 0$. Hence:

$$\mathbf{S}\mathbf{u}^{[2]} = \lambda^{[2]}\mathbf{u}^{[2]}.$$

Similarly, we want to maximise the variance so we select the eigenvector associated with the largest remaining eigenvalue. The solution proceeds in a similar step-wise fashion to give:

$$\left\{\mathbf{u}^{[j]*} = \mathbf{q}_j\right\}_{j=1}^{d}$$

implying a total projected variance of:

$$L^* = \sum_{j=1}^{d} \mathbf{q}_j^T \mathbf{S}\mathbf{q}_j = \sum_{j=1}^{d} \lambda_j.$$

This solution assumes orthogonality of basis vectors, normality of different basis vectors and the orientation of the first basis vector. Other choices are also possible yielding similar solutions. While the original problem is non-convex, it is possible to show that the greedy local optima gives rise to **globally optimal points**.
PCA allows estimation of the input space as the space spanned by the first d eigenvectors with the largest eigenvalues of the sample covariance matrix.

Definition (Ambient and Intrinsic Dimensionalities)**.** The dimensionality of the input space is known as the ambient dimensionality of the data, and the dimensionality of the subspace upon which the data is assumed to lie is known as the intrinsic dimensionality of the data.

Pattern Stabilility

To be sure that the training sample has discerned a reliable subspace (intuitively, how extensible the subspace is to other data) we consider two other approaches:

- **Generative Modelling**: Seeking a Gaussian latent variable model to be learned using MLE or Bayesian treatment
- **PAC Approach**: Bounding generalisation error resulting from projection $E_{\mathcal{D}}\left[\mathbf{x} - \sum_{j=1}^{d}\left(\mathbf{u}^{[j]} \cdot \mathbf{x}\right)\mathbf{u}^{[j]}\right]$ with high probability. Bound consists terms in sample residual eigenspectrum and complexity of data space. With a subspace capturing a high proportion of the variance with a small relative dimensionality, we have low generalisation error.

8.2 Probabilistic PCA

In Probabilistic PCA, we seek a Gaussian latent variable model and learn its parameters as a probabilistic generalisation of PCA.

PPCA Model

We assume that each point has an unknown latent variable $\mathbf{z} \in \mathbb{R}^d$ associated with it corresponding to its position in the principal component subspace. We assume this variable is a outcome of a Gaussian random variable $\mathcal{Z}$:

$$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d).$$

Additionally, each $\mathbf{x}$ is a outcome of a Gaussian random variable $\mathcal{X}$:

$$\mathbf{x}|\mathbf{z} \sim \mathcal{N}\left(\mathbf{W}\mathbf{z} + \mu, \sigma^2 \mathbf{I}_m\right).$$

where $\mathbf{W} \in \mathbb{R}^{m \times d}$ defining the directions of the principal subspace, $\mu \in \mathbb{R}^m, \sigma \in \mathbb{R}^+$.

Intuitively, we can understand the model as follows:

- We draw an outcome for the latent variable $\mathbf{z}$.
- The observed variable is sample conditional on the latent variable $\mathbf{x}|\mathbf{z}$.
- We observe residual noise ε such that:

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \mu + \varepsilon.$$
$$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d).$$
$$\varepsilon \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 \mathbf{I}_m\right).$$

Remark. Given a marginal distribution for $\tilde{\mathbf{x}}$ and a conditional Gaussian distribution for $\tilde{\mathbf{y}}$ given $\tilde{\mathbf{x}}$:

$$\tilde{\mathbf{x}} \sim \mathcal{N}(\mu, \mathbf{\Lambda}^{-1})$$
$$\tilde{\mathbf{y}}|\tilde{\mathbf{x}} \sim \mathcal{N}(\mathbf{A}\tilde{\mathbf{x}} + \mathbf{b}, \mathbf{L}^{-1})$$

for some $\tilde{\mathbf{x}} \in \mathbb{R}^n, \tilde{\mathbf{y}} \in \mathbb{R}^m, \mu \in \mathbb{R}^n, \mathbf{\Lambda} \in \mathbb{R}^{n \times n}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{b} \in \mathbb{R}^m, \mathbf{L} \in \mathbb{R} \in^{m \times m}$. Then:

$$\tilde{\mathbf{y}} \sim \mathcal{N}\left(\mathbf{A}\mu + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1}\mathbf{A}^{\mathbf{T}}\right).$$
$$\tilde{\mathbf{x}}|\tilde{\mathbf{y}} \sim \mathcal{N}(\mathbf{\Sigma}\left[\mathbf{A}^T\mathbf{L}(\tilde{\mathbf{y}} - \mathbf{b}) + \mathbf{\Lambda}\mu\right], \mathbf{\Sigma})$$

where $\Sigma = \left(\mathbf{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)^{-1}$

Given this, we have:

$$\mathbf{x} \sim \mathcal{N}\left(\mu, \mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I}_m\right).$$

Since the covariance matrix of the distribution of $\mathbf{x}$ is symmetric, we can interpret $p_{\mathcal{X}}(\mathbf{x})$ as a density determined by σ^2 of taking an isotropic Gaussian 'spray can' across the principal subspace. We have a 'pancake' shaped distribution.

Rotational Invariance

Suppose $\mathbf{R}$ an orthogonal (rotation) matrix (hence $\mathbf{R}^T\mathbf{R} = \mathbf{I}$). Applying it to the latent space coordinate matrix $\mathbf{W}$:

$$\begin{aligned} \tilde{\mathbf{W}} &= \mathbf{W}\mathbf{R} \\ \implies \tilde{\mathbf{W}}\tilde{\mathbf{W}}^T &= \mathbf{W}\mathbf{R}\mathbf{R}^T\mathbf{W}^T \\ &= \mathbf{W}\mathbf{W}^T \end{aligned}$$

The distribution of $\mathbf{x}$ can be characterised by any $\tilde{\mathbf{W}}$. THis is the analogue of the non-uniqueness in PCA.

Optimisation

We find the log-likelihood function to optimise as follows:

$$\begin{aligned}\mathcal{L} &= \sum_{i=1}^{n} \ln p_{\mathcal{X}} \left(\mathbf{x}^{(i)}; \mathbf{W}, \mu, \sigma^2\right) \\ &= -\frac{nm}{2} \ln(2\pi) - \frac{n}{2} \ln |\mathbf{C}| - \frac{1}{2} \sum_{i=1}^{n} \left(\mathbf{x}^{(i)} - \mu\right)^T \mathbf{C}^{-1} \left(\mathbf{x}^{(i)} - \mu\right)\end{aligned}$$

It can be demonstrated that the following closed form solutions flow from the optimisation of this function (Tipping & Bishop, 1999):

$$\mu_{MLE} = \overline{\mathbf{x}}.$$

$$\sigma_{MLE} = \frac{1}{m-d} \sum_{i=d+1}^{m} \lambda_i.$$

$$\mathbf{W}_{MLE} = \mathbf{Q}\left(\mathbf{\Lambda} - \sigma^2 \mathbf{I}\right)^{\frac{1}{2}\mathbf{R}}.$$

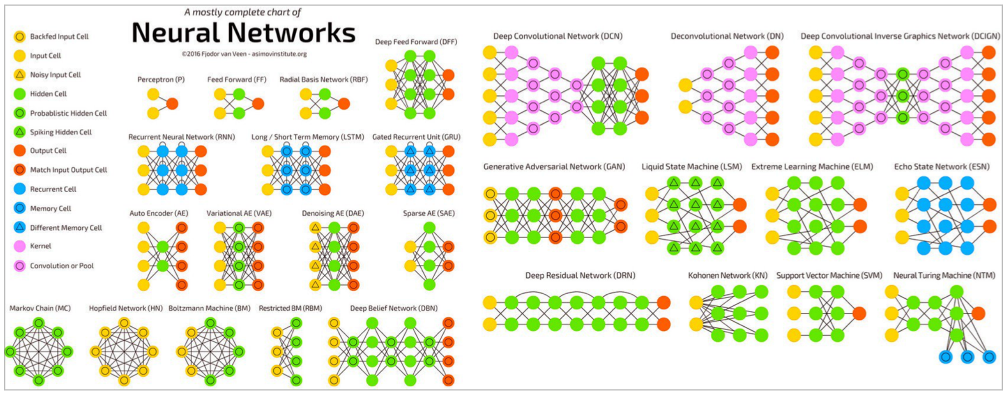
where $\mathbf{Q} \in \mathbb{R}^{m \times d}$ whose columns are given by the leading d eigenvectors of the covariance matrix $\mathbf{S}$, $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$ contains the d eigenvalues associated with these eigenvectors, and $\mathbf{R}$ is an arbitrary orthogonal matrix. We can set $\mathbf{R} = \mathbf{I}$ without loss of generality, when $\mathbf{W}$ are the principal component eigenvectors scaled by the square root of the variance parameters $(\lambda_i - \sigma^2)^{\frac{1}{2}}$. Hence, the variance of $p_{\mathcal{X}}(\mathbf{x})$ in the $\mathbf{q}_i$ direction is λ_i.

9 Neural Networks

Definition (Artificial Neuron)**.** In neural networks, an artificial neuron is a mapping between some inputs $\mathbf{x} \in \mathbb{R}^m \mapsto \mathbb{R}$. It is defined by a weight vector $\mathbf{w}$ and a bias term b, and the sum is passed through an activation function:

$$f(\mathbf{x}) = \hat{\phi}\left(\mathbf{w} \cdot \mathbf{x} + \mathbf{b}\right).$$

Often we take the logistic sigmoid $\hat{\phi}(z) = \frac{1}{1+e^{-z}}$, or the heaviside function. An Artificial Neural Network is a combination of many of these units, how they are connected may be complex and is characterised by the NN's architecture.


A mostly complete chart of
Neural Networks
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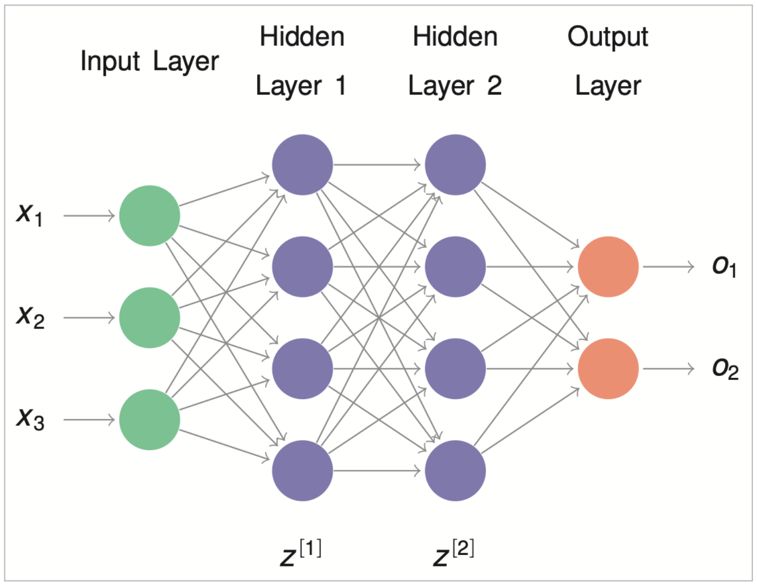
Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)
Markov Chain (MC)
Hopfield Network (HN)
Boltzmann Machine (BM)
Restricted BM (RBM)
Deep Belief Network (DBN)
Deep Convolutional Network (DCN)
Deconvolutional Network (DN)
Deep Convolutional Inverse Graphics Network (DCIGN)
Generative Adversarial Network (GAN)
Liquid State Machine (LSM)
Extreme Learning Machine (ELM)
Echo State Network (ESN)
Deep Residual Network (DRN)
Kohonen Network (KN)
Support Vector Machine (SVM)
Neural Turing Machine (NTM)

We have two broad categories:

- **Feed Forward Neural Networks**: where units are arranged into a graph without any cycles. This exploits the local structure of data, such as in a CNN.
- **Recurrent Neural Networks**: where the graph can have cycles such that outputs of a unit can loop back to become one of its inputs. This may be well used to perceive time series structures.

9.1 Multilayer Perceptron

A particular form of FFN where each layer contains some identical sigmoid units, the Multilayer Perceptron (MLP) is fully connected (every unit in one layer is connected to every layer in the next). We call the first layer the input layer, the last layer the output layer, and those in between



the hidden layers. The number of layers is the depth of the MLP and the number of units in a layer is known as the width of the MLP. We have in general:

$$z_i^{[h]} = \hat{\phi}\left(\sum_j w_{ij}^{[h]} z_j^{h-1} + b_i^{[h]}\right).$$

Feature Learning

A NN is nonlinear mapping between a set of input variables x to a set of output variables $\{o_i\}$ with functional forms controlled by weights $\mathbf{w}$ to learn. Number of weights and basis functions are cosen via our architecture, but they are adaptive through the weights. Features can be learned implicitly with deeper layers learning more complex features.
Due to the non-linearity of activation functions, even a shallow MLP with just one hidden layer can learn any non-linear function of the input. We call MLP a **universal function approximator**, even though it might not be compact.

Evaluation

For a H hidden layer network, we have three canonical cases:

- **Regression**: We have one output to be a linear function of units in the last layer

  $$o^{(i)} = \sum_j w_j^{[H+1]} z_j^{[H](i)} + b^{[H+1]}$$

  and the evaluation function to be the squared loss

  $$L = \frac{1}{2} \sum_{i=1}^{n} \left(o^{(i)-y^{(i)}}\right)^2$$

- **Binary Classification**: We have one output to be a logistic sigmoid function of units in the last layer

  $$o^{(i)} = \frac{1}{1 + e^{-(\sum_j w_j^{[H+1]} z_j^{[H](i)} + b^{[H+1]})}}$$

  and the evaluation function to be the cross entropy

  $$L = -\sum_{i=1}^{n} y^{(i)} \ln(o^{(i)}) + (1 - y^{(i)}) \ln(1 - o^{(i)})$$

- **Multi-Classification**: We have K 'initial' outputs from the last layer

  $$\tilde{o}_k^{(i)} = \sum_j w_j^{[H+1]} z_j^{[H](i)} + b^{[H+1]}$$

  of which we put through a softmax function to generate the final output units:

  $$o_k^{(i)} = \frac{\exp(\tilde{o}_k^{(i)})}{\sum_{j=1}^{K} \exp(\tilde{o}_j^{(i)})}$$

  and the evaluation function to be the cross entropy

  $$L = -\sum_{i=1}^{n} \sum_{k=1}^{K} y_k^{(i)} \ln(\tilde{o}_k^{(i)})$$

We evaluate $o^{(i)}$ for each of the training examples, as a forward pass through the network from th e first hidden layer, second hidden layer and so on. This process is known as the **forward propagation** of information through the network.

Optimisation