



# Signal Processing and Machine Learning

## 1. Math

$\pi \approx 3.141\,59$  $e \approx 2.718\,28$  $\sqrt{2} \approx 1.414$  $\sqrt{3} \approx 1.732$

**Binome, Trinome**  
 $(a \pm b)^2 = a^2 \pm 2ab + b^2$  $a^2 - b^2 = (a - b)(a + b)$   
 $(a \pm b)^3 = a^3 \pm 3a^2b + 3ab^2 \pm b^3$   
 $(a + b + c)^2 = a^2 + b^2 + c^2 + 2ab + 2ac + 2bc$

**Folgen und Reihen**  
 $\sum_{k=1}^n k = \frac{n(n+1)}{2}$  $\sum_{k=0}^n q^k = \frac{1-q^{n+1}}{1-q}$  $\sum_{n=0}^{\infty} \frac{z^n}{n!} = e^z$   
Arithmetrische SummenformelGeometrische SummenformelExponentialreihe

**Mittelwerte** ( $\sum$  von  $i$  bis  $N$ ) (Median: Mitte einer geordneten Liste)  
 $\bar{x}_{ar} = \frac{1}{N} \sum x_i \geq \bar{x}_{geo} = \sqrt[N]{\prod x_i} \geq \bar{x}_{hm} = \frac{N}{\sum \frac{1}{x_i}}$   
ArithmetischesGeometrisches MittelHarmonisches

**Ungleichungen:** Bernoulli-Ungleichung:  $(1+x)^n \geq 1+nx$   
 $||x| - |y|| \leq |x \pm y| \leq |x| + |y|$  $|\underline{x}^T \cdot \underline{y}| \leq \|\underline{x}\| \cdot \|\underline{y}\|$   
DreiecksungleichungCauchy-Schwarz-Ungleichung

**Mengen:** De Morgan:  $\overline{A \cap B} = \overline{A} \cup \overline{B}$  $\overline{A \cup B} = \overline{A} \cap \overline{B}$

**1.1. Exp. und Log.** $e^x := \lim_{n \rightarrow \infty} (1 + \frac{x}{n})^n$  $e \approx 2,71828$   
 $a^x = e^{x \ln a}$  $\log_a x = \frac{\ln x}{\ln a}$  $\ln x \leq x - 1$   
 $\ln(x^a) = a \ln(x)$  $\ln(\frac{x}{a}) = \ln x - \ln a$  $\log(1) = 0$

**1.2. Matrizen**  $\underline{A} \in \mathbb{K}^{m \times n}$   
 $\underline{A} = (a_{ij}) \in \mathbb{K}^{m \times n}$  hat  $m$  Zeilen (Index  $i$ ) und  $n$  Spalten (Index  $j$ )  
 $(\underline{A} + \underline{B})^T = \underline{A}^T + \underline{B}^T$  $(\underline{A} \cdot \underline{B})^T = \underline{B}^T \cdot \underline{A}^T$   
 $(\underline{A}^T)^{-1} = (\underline{A}^{-1})^T$  $(\underline{A} \cdot \underline{B})^{-1} = \underline{B}^{-1} \underline{A}^{-1}$   
 $\dim \mathbb{K} = n = \text{rang } \underline{A} + \dim \ker \underline{A}$  $\text{rang } \underline{A} = \text{rang } \underline{A}^T$

**1.2.1. Quadratische Matrizen**  $\underline{A} \in \mathbb{K}^{n \times n}$   
regulär/invertierbar/nicht-singulär  $\Leftrightarrow \det(\underline{A}) \neq 0 \Leftrightarrow \text{rang } \underline{A} = n$   
singulär/nicht-invertierbar  $\Leftrightarrow \det(\underline{A}) = 0 \Leftrightarrow \text{rang } \underline{A} \neq n$   
orthogonal  $\Leftrightarrow \underline{A}^T = \underline{A}^{-1} \Rightarrow \det(\underline{A}) = \pm 1$   
symmetrisch:  $\underline{A} = \underline{A}^T$ schief-symmetrisch:  $\underline{A} = -\underline{A}^T$

**1.2.2. Determinante von A**  $\in \mathbb{K}^{n \times n}$ :  $\det(\underline{A}) = |\underline{A}|$   
 $\det \begin{bmatrix} \underline{A} & \underline{0} \\ \underline{C} & \underline{D} \end{bmatrix} = \det \begin{bmatrix} \underline{A} & \underline{B} \\ \underline{0} & \underline{D} \end{bmatrix} = \det(\underline{A}) \det(\underline{D})$   
 $\det(\underline{A}) = \det(\underline{A}^T)$  $\det(\underline{A}^{-1}) = \det(\underline{A})^{-1}$   
 $\det(\underline{AB}) = \det(\underline{A}) \det(\underline{B}) = \det(\underline{B}) \det(\underline{A}) = \det(\underline{BA})$   
Hat  $\underline{A}$  2 linear abhäng. Zeilen/Spalten  $\Rightarrow |\underline{A}| = 0$

**1.2.3. Eigenwerte (EW)  $\lambda$  und Eigenvektoren (EV)  $\underline{v}$**   
 **$\underline{A}\underline{v} = \lambda \underline{v}$     $\det \underline{A} = \prod \lambda_i$     $\text{Sp } \underline{A} = \sum a_{ii} = \sum \lambda_i$**

Eigenwerte:  $\det(\underline{A} - \lambda \underline{1}) = 0$  Eigenvektoren:  $\ker(\underline{A} - \lambda_i \underline{1}) = \underline{v}_i$   
EW von Dreieck/Diagonal Matrizen sind die Elem. der Hauptdiagonale.

**1.2.4. Spezialfall  $2 \times 2$  Matrix A**  
 $\det(\underline{A}) = ad - bc$  $\text{Sp}(\underline{A}) = a + d$  $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{\det \underline{A}} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$   
 $\lambda_{1/2} = \frac{\text{Sp } \underline{A}}{2} \pm \sqrt{\left(\frac{\text{Sp } \underline{A}}{2}\right)^2 - \det \underline{A}}$

**1.2.5. Differentiation**  
 $\frac{\partial \underline{x}^T \underline{y}}{\partial \underline{x}} = \frac{\partial \underline{y}^T \underline{x}}{\partial \underline{x}} = \underline{y}$  $\frac{\partial \underline{x}^T \underline{a}}{\partial \underline{x}} = \underline{a}$   
 $\frac{\partial \underline{x}^T \underline{BAx}}{\partial \underline{A}} = \underline{xy}^T$  $\frac{\partial \det(\underline{BAx})}{\partial \underline{A}} = \det(\underline{BAx}) (\underline{A}^{-1})^T$

**1.2.6. Ableitungsregeln** ( $\forall \lambda, \mu \in \mathbb{R}$ )  
Linearität:  $(\lambda f + \mu g)'(x) = \lambda f'(x) + \mu g'(x)$   
Produkt:  $(f \cdot g)'(x) = f'(x)g(x) + f(x)g'(x)$   
Quotient:  $\left(\frac{f}{g}\right)'(x) = \frac{g(x)f'(x) - f(x)g'(x)}{g(x)^2}$  ( $\frac{\text{NAZ}-\text{ZAN}}{\text{N}^2}$ )  
Kettenregel:  $(f(g(x)))' = f'(g(x))g'(x)$

**1.3. Integrale**  $\int e^x dx = e^x = (e^x)'$   
Partielle Integration:  $\int u w' = u w - \int u' w$   
Substitution:  $\int f(g(x))g'(x) dx = \int f(t) dt$

$F(x) - C$	$f(x)$	$f'(x)$
$\frac{1}{q+1} x^{q+1}$	$x^q$	$q x^{q-1}$
$\frac{2\sqrt{ax^3}}{3}$	$\sqrt{ax}$	$\frac{a}{2\sqrt{ax}}$
$x \ln(ax) - x$	$\ln(ax)$	$\frac{1}{x}$
$\frac{1}{a^2} e^{ax} (ax - 1)$	$x \cdot e^{ax}$	$e^{ax} (ax + 1)$
$\frac{a^x}{\ln(a)}$	$a^x$	$a^x \ln(a)$
$-\cos(x)$	$\sin(x)$	$\cos(x)$
$\cosh(x)$	$\sinh(x)$	$\cosh(x)$
$-\ln \cos(x) $	$\tan(x)$	$\frac{1}{\cos^2(x)}$

$\int e^{at} \sin(bt) dt = e^{at} \frac{a \sin(bt) + b \cos(bt)}{a^2 + b^2}$   
 $\int \frac{dt}{\sqrt{at+b}} = \frac{2\sqrt{at+b}}{a}$  $\int t^2 e^{at} dt = \frac{(a-1)^2 + 1}{a^3} e^{at}$   
 $\int t e^{at} dt = \frac{at-1}{a^2} e^{at}$  $\int x e^{ax^2} dx = \frac{1}{2a} e^{ax^2}$

**1.3.1. Volumen und Oberfläche von Rotationskörpern um x-Achse**  
 $V = \pi \int_a^b f(x)^2 dx$  $O = 2\pi \int_a^b f(x) \sqrt{1 + f'(x)^2} dx$

## 2. Probability Theory Basics

**2.1. Kombinatorik**  
Mögliche Variationen/Kombinationen um  $k$  Elemente von maximal  $n$  Elementen zu wählen bzw.  $k$  Elemente auf  $n$  Felder zu verteilen:

	Mit Reihenfolge	Reihenfolge egal
Mit Wiederholung	$n^k$	$\binom{n+k-1}{k}$
Ohne Wiederholung	$\frac{n!}{(n-k)!}$	$\binom{n}{k}$

Permutation von  $n$  mit jeweils  $k$  gleichen Elementen:  $\frac{n!}{k_1! \cdot k_2! \cdot \dots}$   
Binomialkoeffizient  $\binom{n}{k} = \binom{n}{n-k} = \frac{n!}{k! \cdot (n-k)!}$   
 $\binom{n}{0} = 1$  $\binom{n}{1} = n$  $\binom{n}{2} = 6$  $\binom{n}{5} = 10$  $\binom{n}{2} = 15$

**2.2. Der Wahrscheinlichkeitsraum ( $\Omega, \mathbb{F}, \mathbf{P}$ )**

<b>Ergebnismenge</b>	$\Omega = \{\omega_1, \omega_2, \dots\}$	Ergebnis $\omega_j \in \Omega$
<b>Ereignisalgebra</b>	$\mathbb{F} = \{A_1, A_2, \dots\}$	Ereignis $A_i \subseteq \Omega$
<b>Wahrscheinlichkeitsmaß</b>	$\mathbf{P} : \mathbb{F} \rightarrow [0, 1]$	$\mathbf{P}(A) = \frac{ A }{ \Omega }$

**2.3. Wahrscheinlichkeitsmaß P**  
 $\mathbf{P}(A) = \frac{|A|}{|\Omega|}$  $\mathbf{P}(A \cup B) = \mathbf{P}(A) + \mathbf{P}(B) - \mathbf{P}(A \cap B)$

**2.3.1. Axiome von Kolmogorow**  
Nichtnegativität:  $\mathbf{P}(A) \geq 0 \Rightarrow \mathbf{P} : \mathbb{F} \mapsto [0, 1]$   
Normiertheit:  $\mathbf{P}(\Omega) = 1$   
Additivität:  $\mathbf{P}\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} \mathbf{P}(A_i)$ , wenn  $A_i \cap A_j = \emptyset, \forall i \neq j$

**2.4. Bedingte Wahrscheinlichkeit**  
Bedingte Wahrscheinlichkeit für  $A$  falls  $B$  bereits eingetreten ist:  
 $\mathbf{P}_B(A) = \mathbf{P}(A|B) = \frac{\mathbf{P}(A \cap B)}{\mathbf{P}(B)}$

**2.4.1. Totale Wahrscheinlichkeit und Satz von Bayes**  
Es muss gelten:  $\bigcup_{i \in I} B_i = \Omega$  für  $B_i \cap B_j = \emptyset, \forall i \neq j$   
Totale Wahrscheinlichkeit:  $\mathbf{P}(A) = \sum_{i \in I} \mathbf{P}(A|B_i) \mathbf{P}(B_i)$   
Satz von Bayes:  $\mathbf{P}(B_k|A) = \frac{\mathbf{P}(A|B_k) \mathbf{P}(B_k)}{\sum_{i \in I} \mathbf{P}(A|B_i) \mathbf{P}(B_i)}$

**Multiplikationssatz:**  $\mathbf{P}(A \cap B) = \mathbf{P}(A|B) \mathbf{P}(B) = \mathbf{P}(B|A) \mathbf{P}(A)$

**2.5. Zufallsvariable**  
 $X : \Omega \mapsto \Omega'$  ist Zufallsvariable, wenn für jedes Ereignis  $A' \in \mathbb{F}'$  im Bildraum ein Ereignis  $A$  im Urbildraum  $\mathbb{F}$  existiert, sodass  $\{\omega \in \Omega | X(\omega) \in A'\} \in \mathbb{F}$

**2.6. Distribution**

Bezeichnung	Abk.	Zusammenhang
Wahrscheinlichkeitsdichte	pdf	$f_X(x) = \frac{dF_X(x)}{dx}$
Kumulative Verteilungsfkt.	cdf	$F_X(x) = \int_{-\infty}^x f_X(\xi) d\xi$

Joint CDF:  $F_{X,Y}(x, y) = \mathbf{P}(\{X \leq x, Y \leq y\})$

**2.7. Relations between  $f_X(x), f_{X,Y}(x, y), f_{X|Y}(x|y)$**

$$\underbrace{\int_{-\infty}^{\infty} f_{X,Y}(x, \xi) d\xi}_{\text{Marginalization}} = \underbrace{\int_{-\infty}^{\infty} f_{X|Y}(x, \xi) f_Y(\xi) d\xi}_{\text{Total Probability}} = f_X(x)$$

**2.8. Bedingte Zufallsvariablen**  
Ereignis A gegeben:  $F_{X|A}(x|A) = \mathbf{P}(\{X \leq x\} | A)$   
ZV Y gegeben:  $F_{X|Y}(x|y) = \mathbf{P}(\{X \leq x\} | \{Y = y\})$   
 $p_{X|Y}(x|y) = \frac{p_{X,Y}(x, y)}{p_Y(y)}$   
 $f_{X|Y}(x|y) = \frac{f_{X,Y}(x, y)}{f_Y(y)} = \frac{dF_{X|Y}(x|y)}{dx}$

**2.9. Unabhängigkeit von Zufallsvariablen**  
 $X_1, \dots, X_n$  sind stochastisch unabhängig, wenn für jedes  $\underline{x} \in \mathbb{R}^n$  gilt:  
 $F_{X_1, \dots, X_n}(x_1, \dots, x_n) = \prod_{i=1}^n F_{X_i}(x_i)$   
 $p_{X_1, \dots, X_n}(x_1, \dots, x_n) = \prod_{i=1}^n p_{X_i}(x_i)$   
 $f_{X_1, \dots, X_n}(x_1, \dots, x_n) = \prod_{i=1}^n f_{X_i}(x_i)$

## 3. Gaussian Stuff

**3.1. Gaussian Channel**  
Channel:  $Y = h s_i + N$  with  $h \sim \mathcal{N}, N \sim \mathcal{N}$   
 $L(y_1, \dots, y_N) = \prod_{i=1}^N f_{Y_i}(y_i, h)$   
 $f_{Y_i}(y_i, h) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y_i - h s_i)^2\right)$   
 $\hat{h}_{ML} = \underset{h}{\text{argmin}} \left\{ \left\| \underline{y} - h \underline{s} \right\|^2 \right\} = \frac{\underline{s}^T \underline{y}}{\underline{s}^T \underline{s}}$   
If multidimensional channel:  $\underline{y} = \underline{S} \underline{h} + \underline{n}$ :  
 $L(\underline{y}, \underline{h}) = \frac{1}{\sqrt{\det(2\pi \underline{C})}} \exp\left(-\frac{1}{2}(\underline{y} - \underline{S} \underline{h})^T \underline{C}^{-1}(\underline{y} - \underline{S} \underline{h})\right)$   
 $l(\underline{y}, \underline{h}) = \frac{1}{2} \left( \log(\det(2\pi \underline{C})) - (\underline{y} - \underline{S} \underline{h})^T \underline{C}^{-1}(\underline{y} - \underline{S} \underline{h}) \right)$   
 $\frac{d}{d\underline{h}} (\underline{y} - \underline{S} \underline{h})^T \underline{C}^{-1}(\underline{y} - \underline{S} \underline{h}) = -2 \underline{S}^T \underline{C}^{-1}(\underline{y} - \underline{S} \underline{h})$   
**Gaussian Covariance:** if  $Y \sim \mathcal{N}(0, \sigma^2), N \sim \mathcal{N}(0, \sigma^2)$ :  
 $\underline{C}_Y = \text{Cov}[Y, Y] = \mathbb{E}[(Y - \mu)(Y - \mu)^T] = \mathbb{E}[Y Y^T]$   
For Channel  $Y = S h + N$ :  $\mathbb{E}[Y Y^T] = S \mathbb{E}[h h^T] S^T + \mathbb{E}[N N^T]$

**3.2. Multivariate Gaussian Distributions**  
A vector  $\underline{x}$  of  $n$  independent Gaussian random variables  $x_i$  is jointly Gaussian. If  $\underline{x} \sim \mathcal{N}(\underline{\mu}_{\underline{x}}, \underline{C}_{\underline{x}})$ :

$$f_{\underline{x}}(\underline{x}) = f_{x_1, \dots, x_n}(x_1, \dots, x_n) = \frac{1}{\sqrt{\det(2\pi \underline{C}_{\underline{x}})}} \exp\left(-\frac{1}{2}(\underline{x} - \underline{\mu}_{\underline{x}})^T \underline{C}_{\underline{x}}^{-1}(\underline{x} - \underline{\mu}_{\underline{x}})\right)$$

Affine transformations  $\underline{y} = \underline{A} \underline{x} + \underline{b}$  are jointly Gaussian with  $\underline{y} \sim \mathcal{N}(\underline{A} \underline{\mu}_{\underline{x}} + \underline{b}, \underline{A} \underline{C}_{\underline{x}} \underline{A}^T)$   
All marginal PDFs are Gaussian as well  
**Contour Lines**  
Ellipsoid with central point  $\mathbb{E}[\underline{y}]$  and main axis are the eigenvectors of  $\underline{C}_{\underline{y}}^{-1}$

**3.3. Conditional Gaussian**  
 $\underline{A} \sim \mathcal{N}(\underline{\mu}_{\underline{A}}, \underline{C}_{\underline{A}}), \underline{B} \sim \mathcal{N}(\underline{\mu}_{\underline{B}}, \underline{C}_{\underline{B}})$   
 $\Rightarrow (\underline{A} | \underline{B} = \underline{b}) \sim \mathcal{N}(\underline{\mu}_{\underline{A}|\underline{B}}, \underline{C}_{\underline{A}|\underline{B}})$   
**Conditional Mean:**  
 $\mathbb{E}[\underline{A} | \underline{B} = \underline{b}] = \underline{\mu}_{\underline{A}|\underline{B}=\underline{b}} = \underline{\mu}_{\underline{A}} + \underline{C}_{\underline{AB}} \underline{C}_{\underline{BB}}^{-1} (\underline{b} - \underline{\mu}_{\underline{B}})$   
**Conditional Variance:**  
 $\underline{C}_{\underline{A}|\underline{B}} = \underline{C}_{\underline{AA}} - \underline{C}_{\underline{AB}} \underline{C}_{\underline{BB}}^{-1} \underline{C}_{\underline{BA}}$

**3.4. Misc**  
If CDF of gaussian distribution given  $\Phi(z) \sim \mathcal{N}(0, 1)$  then for  $X \sim \mathcal{N}(1, 1)$  the CDF is given as  $\Phi(x - \mu_x)$

## 4. Common Distributions

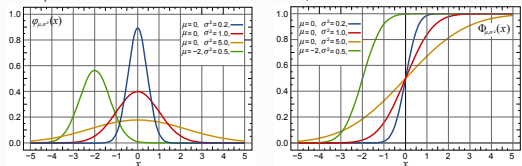
**4.1. Binomialverteilung  $\mathcal{B}(n, p)$  mit  $p \in [0, 1], n \in \mathbb{N}$**   
Folge von  $n$  Bernoulli-Experimenten  
 $p$ : Wahrscheinlichkeit für Erfolg    $k$ : Anzahl der Erfolge  
 $p_X(k) = B_{n,p}(k) = \begin{cases} \binom{n}{k} p^k (1-p)^{n-k} & k \in \{0, \dots, n\} \\ 0 & \text{sonst} \end{cases}$

$\mathbb{E}[X] = np$ Erwartungswert	$\text{Var}[X] = np(1-p)$ Varianz	$G_X(z) = (pz + 1 - p)^n$ Wahrscheinlichkeitserz. Funktion
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## 4.2. Normalverteilung

WDF/PDF:

KVF/CDF:



$$\text{WDF: } f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad x \in \mathbb{R} \quad \begin{matrix} \mu \in \mathbb{R} \\ \sigma > 0 \end{matrix}$$

$$\begin{matrix} E(X) = \mu & \text{Var}(X) = \sigma^2 & \varphi_X(\omega) = e^{j\omega\mu - \frac{\omega^2\sigma^2}{2}} \\ \text{Erwartungswert} & \text{Varianz} & \text{Charakt. Funktion} \end{matrix}$$

## 4.3. Sonstiges

**Gamma**distribution  $\Gamma(\alpha, \beta)$ :  $E[X] = \frac{\alpha}{\beta}$

**Exponential**:  $f(x, \lambda) = \lambda e^{-\lambda x}$   $E[X] = \lambda^{-1}$   $\text{Var}[X] = \lambda^{-2}$

## 5. Wichtige Parameter

### 5.1. Erwartungswert (1. zentrales Moment)

gibt den mittleren Wert einer Zufallsvariablen an

$$\mu_X = E[X] = \sum_{x \in \Omega'} x \cdot P_X(x) \triangleq \int_{\mathbb{R}} x \cdot f_X(x) dx$$

diskrete  $X: \Omega \rightarrow \Omega'$       stetige  $X: \Omega \rightarrow \mathbb{R}$

$E[\alpha X + \beta Y] = \alpha E[X] + \beta E[Y]$   $X \leq Y \Rightarrow E[X] \leq E[Y]$   
 $E[X^2] = \text{Var}[X] + E[X]^2$   
 $E[X Y] = E[X] E[Y]$ , falls  $X$  und  $Y$  stochastisch unabhängig  
 Umkehrung nicht möglich: Unkorreliertheit  $\nRightarrow$  Stoch. Unabhängig!

#### 5.1.1. Für Funktionen von Zufallsvariablen $g(x)$

$$E[g(X)] = \sum_{x \in \Omega'} g(x) P_X(x) \triangleq \int_{\mathbb{R}} g(x) f_X(x) dx$$

### 5.2. Varianz (2. zentrales Moment)

ist ein Maß für die Stärke der Abweichung vom Erwartungswert

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

$$\text{Var}[\alpha X + \beta] = \alpha^2 \text{Var}[X] \quad \text{Var}[X] = \text{Cov}[X, X]$$

$$\text{Var}\left[\sum_{i=1}^n X_i\right] = \sum_{i=1}^n \text{Var}[X_i] + \sum_{i \neq j} \text{Cov}[X_i, X_j]$$

**Standard Abweichung**:  $\sigma = \sqrt{\text{Var}[X]}$

### 5.3. Kovarianz

Maß für den linearen Zusammenhang zweier Variablen

$$\begin{aligned} \text{Cov}[X, Y] &= E[(X - E[X])(Y - E[Y])^T] = \\ &= E[X Y^T] - E[X] E[Y]^T = \text{Cov}[Y, X] \end{aligned}$$

$$\begin{aligned} \text{Cov}[\alpha X + \beta, \gamma Y + \delta] &= \alpha \gamma \text{Cov}[X, Y] \\ \text{Cov}[X + U, Y + V] &= \text{Cov}[X, Y] + \text{Cov}[X, V] + \text{Cov}[U, Y] + \text{Cov}[U, V] \end{aligned}$$

#### 5.3.1. Korrelation = standardisierte Kovarianz

$$\rho(X, Y) = \frac{\text{Cov}[X, Y]}{\sqrt{\text{Var}[X] \cdot \text{Var}[Y]}} = \frac{C_{xy}}{\sigma_x \sigma_y} \quad \rho(X, Y) \in [-1; 1]$$

#### 5.3.2. Kovarianzmatrix für $\underline{z} = (\underline{x}, \underline{y})^T$

$$\text{Cov}[\underline{z}] = \underline{C}_{\underline{z}} = \begin{bmatrix} C_X & C_{XY} \\ C_{XY}^T & C_Y \end{bmatrix} = \begin{bmatrix} \text{Cov}[X, X] & \text{Cov}[X, Y] \\ \text{Cov}[Y, X] & \text{Cov}[Y, Y] \end{bmatrix}$$

Immer symmetrisch:  $C_{xy} = C_{yx}^T$ ! Für Matrizen:  $\underline{C}_{\underline{x}\underline{y}} = \underline{C}_{\underline{y}\underline{x}}^T$

## 6. Statistical Learning

### 6.1. Definition

**Statistical Model**

Statistical Model:  $\{\mathbb{X}, \mathbb{F}, P_\theta; \theta \in \Theta\}$   
 Sample Space:  $\Omega$   
 Observation Space:  $\mathbb{X}$   
 Sigma Algebra:  $\mathbb{F}$   
 Probability:  $P_\theta$   
 Test (decision rule):  $T: \mathbb{X} \mapsto \{\theta_0, \theta_1\}, x \mapsto T(x)$   
 Null Hypothesis:  $H_0: \theta \in \Theta_0$   
 Alternative Hypothesis:  $H_1: \theta \in \Theta_1$

**Cost Criterion  $G_T$** :

$$\begin{aligned} G_T: \{\theta_0, \theta_1\} &\mapsto [0, 1], \theta \mapsto P(\{T(X) = 1\}; \theta) \\ &= E[T(X); \theta] = \int_{\mathbb{X}} T(x) f_X(x; \theta) dx \end{aligned}$$

**Error Level  $\alpha$** :  $G_T(\theta_0) \leq \alpha$

**Two Error Types**:

False Alarm:  $\theta = \theta_0, T(x) = 1$   
 $G_T(\theta_0) = P(\{T(X) = 1\}; \theta_0)$   
 Detection Error:  $\theta = \theta_1, T(x) = 0$   
 $1 - G_T(\theta_1) = P(\{T(X) = 0\}; \theta_1)$

### 6.2. Maximum Likelihood Test

**ML Ratio Test Statistic (Likelihood Ratio)**:

$$R(x) = \begin{cases} \frac{f_X(x; \theta_1)}{f_X(x; \theta_0)} & ; f_X(x; \theta_0) > 0 \\ \infty & ; f_X(x; \theta_0) = 0 \text{ and } f_X(x; \theta_1) > 0 \end{cases}$$

**ML Test**:

$$T_{ML}: \mathbb{X} \mapsto \{0, 1\}, x \mapsto \begin{cases} 1 & ; R(x) > c = 1 \\ 0 & ; \text{otherwise} \end{cases}$$

if  $R(x)$  is monotonous then it is possible to make a decision by directly comparing  $x$  to a threshold  $x_\alpha$  and every  $R(x) \geq c(\alpha)$  will lead to a unique threshold for  $x_\alpha < x$   
 if  $c \neq 1$  False Alarm Error Probability can be adjusted  $\rightarrow$  Neyman Pearson Test

### 6.3. Neyman-Pearson-Test

minimizes the detection error, while fulfilling a predefined error level  $\alpha$   
 $\arg\max_{d_{NP}} E[d_{NP}(x)|\theta = \theta_1] \quad \text{s.t.} \quad E[d_{NP}(x)|\theta = \theta_0] \leq \alpha$

NP-Test to the error level  $\alpha$ :

$x_\alpha$  is chosen as:  $x_\alpha = (1 - \alpha)$ -quantile of  $f_X(x; \theta_0)$

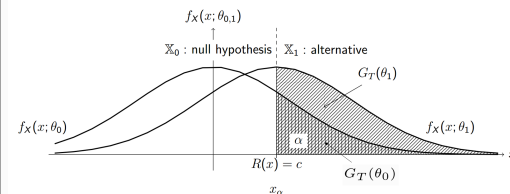
if  $P(\{R(x) = c; \theta_0\}) = 0 \Leftrightarrow$  (if  $x$  is continuous):

$$T_{NP}(x) = \begin{cases} 1 & R(x) > c \\ 0 & R(x) < c \end{cases} \quad \text{Likelihood-Ratio: } R(x) = \frac{f_X(x; \theta_1)}{f_X(x; \theta_0)}$$

if  $P(\{R(x) = c; \theta_0\}) > 0$ :

$$T_{NP}(x) = \begin{cases} 1 & R(x) > c \\ \gamma & R(x) = c, \quad (\text{randomized decision}) \\ 0 & R(x) < c \end{cases}$$

with  $\gamma = \frac{\alpha - P(\{R(x) > c; \theta_0\})}{P(\{R(x) = c; \theta_0\})}$  error level  $\alpha$



**Maximum Likelihood Detector**:  $T_{ML}(x) = \begin{cases} 1 & R(x) > 1 \\ 0 & \text{otherwise} \end{cases}$

**ROC Graphs**: plot  $G_T(\theta_1)$  as a function of  $G_T(\theta_0)$

### 6.4. Bayes Test (MAP Test)

Prior knowledge about possible hypotheses:

$$P(\{\theta \in \Theta_0\}) + P(\{\theta \in \Theta_1\}) = 1$$

$$T_{\text{Bayes}} = \underset{T}{\text{argmin}} \{P_\epsilon\} = \begin{cases} 1 & ; \frac{f_X(x|\theta_1)}{f_X(x|\theta_0)} > c = \frac{P(\theta_0)}{P(\theta_1)} \\ 0 & ; \text{otherwise} \end{cases}$$

$$= \begin{cases} 1 & ; P(\theta_1|x) > P(\theta_0|x) \\ 0 & ; \text{otherwise} \end{cases}$$

with :

$$P_\epsilon = P(\theta_0)G_T(\theta_0) + P(\theta_1)(1 - G_T(\theta_1))$$

if  $P(\theta_0) = P(\theta_1) \rightarrow T_{\text{Bayes}} = T_{ML}$

**Multiple Hypothesis**  $\{\theta_0, \dots, \theta_k\}; \mathbb{X}_0, \dots, \mathbb{X}_k \in \mathbb{X}$ :

$$T_{\text{Bayes}} = \underset{k \in 1, \dots, K}{\text{argmin}} \{P(\theta_k|x)\}$$

**Loss Function**:

$$L(T(x), \theta) = \begin{cases} L_0 & ; T(x) = 1, \text{ but } \theta = \theta_0 \quad (\text{FALSE ALARM}) \\ L_1 & ; T(x) = 0, \text{ but } \theta = \theta_1 \quad (\text{DETEC. ERROR}) \\ 0 & ; \text{otherwise} \end{cases}$$

$L_i$  denotes the Loss Value in cases where the correct decision parameter  $\theta_i$  is missed.

$$\text{Risk}(T) = E[L(T(X), \theta)] = E[E[L(T(x), \theta)|x = X]]$$

### 6.5. Linear Alternative Tests

Estimate normal vector  $\underline{w}^T$  and  $w_0$ , which separate  $\mathbb{X}$  into  $\mathbb{X}_0$  and  $\mathbb{X}_1$   
 $\log R(\underline{x}) = -\frac{1}{2} \ln \left( \frac{\det(\underline{C}_1)}{\det(\underline{C}_0)} \right) - \frac{1}{2} (\underline{x} - \underline{\mu}_1)^T \underline{C}_1^{-1} (\underline{x} - \underline{\mu}_1) + \frac{1}{2} (\underline{x} - \underline{\mu}_0)^T \underline{C}_0^{-1} (\underline{x} - \underline{\mu}_0) = \ln \left( \frac{P(\theta \in \Theta_0)}{P(\theta \in \Theta_1)} \right)$  (separating surface)

For Gaussian  $f_X(x; \mu_k, C_k)$  with  $\theta_0$  and  $\theta_1$  corresponding to  $\{\mu_0, C_0\}$  and  $\{\mu_1, C_1\}$ , it follows that

- if  $C_0 \neq C_1$ ,  $\log R(x) = 0$  is non-linear and the separating surfaces are surfaces of second order: parabolic, hyperbolic, or elliptic surfaces.

- if  $C_0 = C_1$ ,  $\log R(x) = 0$  is affine and thus defines a hyperplane in  $\mathbb{X}$  which decomposes  $\mathbb{X}$  into  $\mathbb{X}_0$  and  $\mathbb{X}_1$ , i.e.,

$$T: \mathbb{X} \mapsto \mathbb{R}, \underline{x} \mapsto \begin{cases} 1 & \underline{w}^T \underline{x} > w_0 \\ 0 & \text{otherwise} \end{cases}$$

case 1:  $\underline{C}_0 = \underline{C}_1 = \sigma^2 \underline{I}_N$

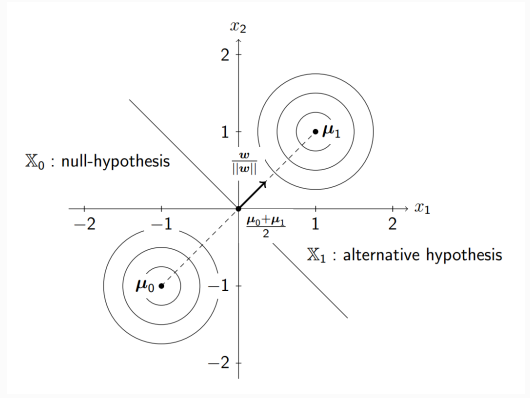
$$\begin{aligned} \underline{w}^T &= (\underline{\mu}_1 - \underline{\mu}_0)^T, \\ w_0 &= \frac{1}{2} (\underline{\mu}_1^T \underline{\mu}_1 - \underline{\mu}_0^T \underline{\mu}_0) - \sigma^2 \ln \left( \frac{P(\theta \in \Theta_1)}{P(\theta \in \Theta_0)} \right) \\ \underline{w} &\text{ colinear with } (\underline{\mu}_1 - \underline{\mu}_0) \\ &\rightarrow \text{hyperplane orthogonal to } (\underline{\mu}_1 - \underline{\mu}_0) \end{aligned}$$

case 2:  $\underline{C}_0 = \underline{C}_1 = \underline{C}$

$$\begin{aligned} \underline{w}^T &= (\underline{\mu}_1 - \underline{\mu}_0)^T \underline{C}^{-1}, \\ w_0 &= \frac{1}{2} (\underline{\mu}_1 - \underline{\mu}_0)^T \underline{C}^{-1} (\underline{\mu}_1 + \underline{\mu}_0) - \ln \left( \frac{P(\theta \in \Theta_1)}{P(\theta \in \Theta_0)} \right) \\ &\text{in general } \underline{w} \text{ not colinear with } (\underline{\mu}_1 - \underline{\mu}_0) \\ &\rightarrow \text{hyperplane not orthogonal to } (\underline{\mu}_1 - \underline{\mu}_0) \end{aligned}$$

- if  $C_0 = C_1$  and  $\mu_0 = -\mu_1$ ,  $\log R(x) = 0$  is linear and defines a separating hyperplane in  $\mathbb{X}$  which contains the origin, i.e.,

$$T: \mathbb{X} \mapsto \mathbb{R}, \underline{x} \mapsto \begin{cases} 1 & \underline{w}^T \underline{x} > 0 \\ 0 & \text{otherwise} \end{cases}$$



## 7. Hypothesis Testing

making a decision based on the observations

### 7.1. Definition

Null hypothesis  $H_0: \theta \in \Theta_0$  (Assumed first to be true)

Alternate hypothesis  $H_1: \theta \in \Theta_1$  (The one to proof)

Decision rule  $\varphi: \mathbb{X} \rightarrow [0, 1]$  with  $\varphi(x) = 1$ : decide for  $H_1$ ,  $\varphi(x) = 0$ : decide for  $H_0$  Error level  $\alpha$  with  $E[d(X)|\theta] \leq \alpha, \forall \theta \in \Theta_0$

Error Type	Decision \ Reality	$H_1$ false ( $H_0$ true)	$H_1$ true ( $H_0$ false)
1 (FA) False Alarm	$H_1$ rejected ( $H_0$ accepted)	True Negative $P = 1 - \alpha$	False Positive (Type 1) $P = \beta$
2 (DE) Detection Error	$H_1$ accepted ( $H_0$ rejected)	False Negative (Type 2) $P = 1 - \beta$	True Positive $P = 1 - \alpha$

Power: Sensitivity/Recall/Hit Rate:  $\frac{TP}{TP+FN} = 1 - \beta$

Specificity/True negative rate:  $\frac{TN}{FP+TN} = 1 - \alpha$

Precision/Positive Prediction rate:  $\frac{TP}{TP+FP}$

Accuracy:  $\frac{TP+TN}{P+N} = \frac{2-\alpha-\beta}{2}$

#### 7.1.1. Design of a test

Cost criterion  $G_\varphi: \Theta \rightarrow [0, 1], \theta \mapsto E[d(X)|\theta]$

False Positive lower than  $\alpha$ :  $G_d(\theta)|_{\theta \in \Theta_0} \leq \alpha, \forall \theta \in \Theta_0$

False Negative small as possible:  $\max\{G_d(\theta)|_{\theta \in \Theta_1}\}, \forall \theta \in \Theta_1$

### 7.2. Sufficient Statistics

Sufficiency for a test  $T(X)$  means that no other test statistic, i.e., function of the observations  $\underline{x}$ , contains additional information about the parameter  $\theta$  to be estimated:

$$f_{X|T}(x|T(x) = t, \theta) = f_X(x|T(x) = t)$$

## 8. Support Vector Machines

### Motivation and Background

#### 8.1. Kernel Methods

Kernel Methods is non-parametric estimation, these make no assumption on statistical model  $\rightarrow$  purely Data-Based.

$$\text{Test Statistic } \mathbb{X} \rightarrow \mathbb{R}, \mathbf{x} \mapsto S(\mathbf{x}) = \sum_{k=1}^M \lambda_k g(\mathbf{x}, \mu_k)$$

linear combination of Kernel Function  $g(\cdot, \mu_k)$ .  $g(\cdot)$  generally non-linear pos. definite

$\mu_k$ : representative for Sample Set  $\mathbb{S} = \{x_1, \dots, x_M\}$   
 $\lambda_k$ : weight coefficient determined by learning  
 Sample Set  $\mathbb{S}$  is Empirical Characterization of Unknown Statistical Model  
 Inference of  $\lambda_k$  based on Sample Set or Training Set is called **Learning**

#### 8.2. Kernel Tests

Statistical Hypothesis Test, where a Sufficient Test Statistic is compared to threshold (i.e.  $R(x) \geq c$ ) decomposes sample space  $\mathbb{X}$  into two disjoint subsets ( $\mathbb{X} = \mathbb{X}_0 \cup \mathbb{X}_1$ )

Separating surface between  $\mathbb{X}_0$  and  $\mathbb{X}_1$  given by:  
 $\{\mathbf{x} | R(\mathbf{x}) = c\}$  The relative position of a sample  $x_j$  to the separating surface determines choice of hypothesis

$$\mathbb{S} = \{(x_1, y_1), \dots, (x_M, y_M)\}$$

$x_i \in \mathbb{R}^N$ ,  $y_i \in \{\Theta_0, \Theta_1\}$   
 Inference of Hypothesis Test based on a Sample Set that includes Labeling  $y_i$  of the elements  $x_i$  is called **Supervised Learning**

Size M of samples has to satisfy:  $M \geq \dim(\mathbb{X})$

Because underlying statistical model is unknown, true  $\theta_0$  and  $\theta_1$  irrelevant  $\rightarrow$  replace them by e.g. -1,+1 for decision between hypotheses

#### 8.3. Linear Kernels

Test Statistic for linear test

$$S(x) = \sum_{i=1}^M \lambda_i \mathbf{x}_i^T \mathbf{x} + w_0 = \mathbf{w}^T \mathbf{x} + w_0 \quad \mathbf{w} = \sum_{i=1}^M \lambda_i \mathbf{x}_i$$

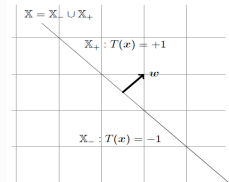
Hyperplane defined by  $\mathbf{w}$  (normal vector or weight vector) and  $w_0$  approximates separating surface between  $\mathbb{X}_-$  and  $\mathbb{X}_+$

$\rightarrow$  Decision rule  $T(\mathbf{x})$ :

$$T(\mathbf{x}) = \text{sign}(S(\mathbf{x})) = \begin{cases} +1 & ; \quad \mathbf{w}^T \mathbf{x} + w_0 \geq 0 \\ -1 & ; \quad \text{otherwise} \end{cases}$$

Linear Kernel Test in sample space  $\mathbb{X}$ :

(Orientation of  $\mathbf{w}$  chosen such that  $\mathbf{w}$  points into direction of  $\Theta_1$  ("+" hypothesis))



To determine  $\mathbf{w}$  and  $w_0$  formulate problem as constrained optimization problem with the constraints:

$\forall k \in \{1, \dots, M\} : T(\mathbf{x}_k) = y_k$

$$\Rightarrow \text{Support Vector Methods: } y_k (\mathbf{w}^T \mathbf{x}_k + w_0) \geq \epsilon, \forall k$$

Robust solution: maximize margin  $\epsilon$  for constant norm of  $\mathbf{w}$

### Application

#### 8.4. Support Vector Methods

only feasible for normalized weight vectors

$$\max_{\mathbf{w}} \epsilon \text{ s.t. } y_k \frac{\mathbf{w}^T}{\|\mathbf{w}\|_2} \mathbf{x}_k \geq \epsilon, \forall k, \quad w_0 = 0$$

$$\Leftrightarrow \min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|_2^2 \text{ s.t. } y_k \mathbf{w}^T \mathbf{x}_k \geq 1, \forall k$$

Optimization Problem convex  $\rightarrow$  **Langragian Method**

$$\text{Dual Problem: } \max_{\mathbf{u}} \min_{\mathbf{w}} \Phi(\mathbf{w}, \mathbf{u}) \text{ s.t. } \mathbf{u} \geq 0$$

Langragian Multiplier:  $u_k \geq 0$

$$\text{Langragian Fct: } \Phi(\mathbf{w}, \mathbf{u}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + \sum_{k=1}^M u_k (1 - y_k \mathbf{w}^T \mathbf{x}_k)$$

$$\frac{\partial \Phi(\mathbf{w}, \mathbf{u})}{\partial \mathbf{w}} \Big|_{\mathbf{w}=\mathbf{w}(\mathbf{u})} = 0 \Leftrightarrow \mathbf{w}(\mathbf{u}) = \sum_{k=1}^M \underbrace{u_k y_k}_{\lambda_k} \mathbf{x}_k$$

Evaluate dual function:

$$\begin{aligned} \Phi(\mathbf{w}(\mathbf{u}), \mathbf{u}) &= \Phi\left(\sum_{k=1}^M u_k y_k \mathbf{x}_k, u_1, \dots, u_M\right) \\ &= -\frac{1}{2} \sum_{k=1}^M \sum_{l=1}^M u_k u_l y_k y_l \mathbf{x}_k^T \mathbf{x}_l + \sum_{k=1}^M u_k \\ &= -\frac{1}{2} \mathbf{u}^T \mathbf{Y} \mathbf{X} \mathbf{X}^T \mathbf{Y} \mathbf{u} + \mathbf{1}^T \mathbf{u} \end{aligned}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_M^T \end{bmatrix}, \mathbf{Y} = \begin{bmatrix} y_1 & & \\ & \ddots & \\ & & y_M \end{bmatrix}, \mathbf{1} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Alternativ to approach above:

**Iterative Solution:**

Choose one element  $\mathbf{x}_k$  out of sample set  $\mathbb{S} = \{\mathbf{x}_1, \dots, \mathbf{x}_M\}$  and randomly set:

$$u_k \leftarrow u_k + \max\{y_k \frac{\partial \Phi(\mathbf{u})}{\partial u_k}, -u_k\}, \forall k$$

Necessary and sufficient condition for existence of solution given by:

$$\mathbf{1} \in \text{conce}[\mathbf{Y} \mathbf{X} \mathbf{X}^T \mathbf{Y}]$$

#### 8.5. Suport Vectors

$$\text{Dual OP: } \max_{\mathbf{u}} \sum_{k=1}^M (-\frac{1}{2} \sum_{l=1}^M u_k u_l y_k y_l \mathbf{x}_k^T \mathbf{x}_l + u_k) \text{ s.t. } u_k \geq 0$$

**Optimal Dual Variables**  $u_1^*, \dots, u_M^*$  either active  $u_k > 0$  or inactive  $u_k = 0$

Elements of  $\mathbb{S}$  with active dual variables = **Support Vectors**

$$\mathbb{S}_{SV} = \{\mathbf{x}_k \in \mathbb{S} | u_k^* > 0\}$$

Elements with inactive dual variables dont contribute to Kernel Test

**Optimal Weight Vektor**  $\mathbf{w}^* = \mathbf{w}(\mathbf{u}^*)$  of Kernel Test constructed by

$$\text{Support Vectors only: } \mathbf{w}^* = \sum_{\mathbf{x}_k \in \mathbb{S}_{SV}} u_k^* y_k \mathbf{x}_k$$

Number of Support Vectors approx. size of  $\dim[\mathbb{X}] \rightarrow$  selection of Support Vectors reduces computational complexity of Kernel Test

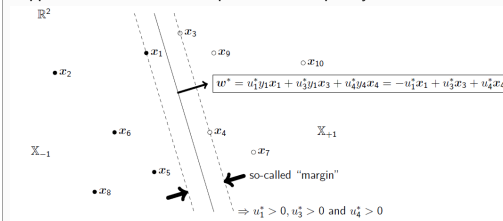


Fig. 2.2: The elements  $x_k \in \mathbb{S}$  with ACTIVE DUAL VARIABLES  $u_k^* > 0$  are called SUPPORT VECTORS.

#### Discussion

- Exists only if  $\mathbb{S}$  **Linearly Separable**
- $w_0 \neq 0$  no (straightforward) iterative solution available
- if **Linearly Inseparable** method generalized by slack variables for controlled violation of constraints

$\rightarrow$  instead of  $\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^T \mathbf{w}$  s.t.  $y_k \mathbf{w}^T \mathbf{x}_k \geq 1$  we get  
 $\min_{\mathbf{w}, \epsilon} \frac{1}{2} \mathbf{w}^T \mathbf{w} + \rho \sum_{k=1}^M \epsilon_k$  s.t.  $y_k \mathbf{w}^T \mathbf{x}_k \geq 1 - \epsilon_k, \forall k, \epsilon, \rho \geq 0$

#### 8.6. Kernel Trick

**Linear Hypothesis Test** often not sufficient  $\rightarrow$  **Kernel Trick**: Generalize linear methods to non-linear approximation of separating surfaces ( $\{\mathbf{x} | \log R(\mathbf{x}) = c\}$ )

Basic Idea: Transfer problem statement into higher-dimensional space (without introducing additional degrees of freedom) by **Feature Map**  $\varphi : \mathbb{S} \rightarrow \mathbb{S}_\varphi$

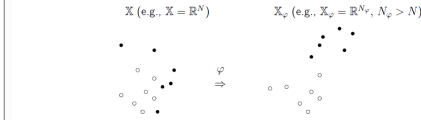


Fig. 2.3: Transfer the problem statement into a higher-dimensional (inner product) space without introducing additional degrees of freedom by means of a so-called FEATURE MAP  $\varphi : \mathbb{S} \rightarrow \mathbb{S}_\varphi$ .

Construction of Linear Test in  $\mathbb{R}^3$  correspondes to Non-Linear Test in  $\mathbb{R}^2$

$$T : \mathbb{R}^3 \rightarrow \{-1, +1\}, \varphi(\mathbf{x}) \mapsto \begin{cases} +1; & \mathbf{w}_\varphi^T \varphi(\mathbf{x}) \geq 0 \\ -1; & \text{otherwise} \end{cases}$$

Linear kernel in  $\mathbb{X}_\varphi$  represents nonlinear kernel in  $\mathbb{X} \rightarrow$  choose Kernel Funktion  $g(\cdot, \cdot)$  directly instead of finding appropriate transformation  $\varphi$

$$\langle \varphi(\mathbf{x}), \varphi(\mathbf{y}) \rangle =: g(\mathbf{x}, \mathbf{y})$$

In Optimization Problem and resulting Dual Function and Variables

$$\text{replace } \mathbf{x} \text{ by } \varphi(\mathbf{x}_k) \rightarrow \text{Dual OP: } \max_{\mathbf{u} \geq 0} \{-\mathbf{u}^T \mathbf{Y} \mathbf{G} \mathbf{Y} \mathbf{u} + \mathbf{1}^T \mathbf{u}\}$$

$$\text{Kernel Matrix } \mathbf{G} = \begin{bmatrix} g(\mathbf{x}_1, \mathbf{x}_2) & \dots & g(\mathbf{x}_1, \mathbf{x}_M) \\ \vdots & & \vdots \\ g(\mathbf{x}_M, \mathbf{x}_1) & \dots & g(\mathbf{x}_M, \mathbf{x}_M) \end{bmatrix} \in \mathbb{R}^{M \times M}$$

After applying **Kernel Trick**: OP and Nonlinear Test  $T$  only based on Kernel Function  $g$ , transformation  $\varphi$  becomes obsolete

$$\text{Hypothesis Test (nonlinear): } T : \mathbf{x} \mapsto \text{sign}\left(\sum_{k=1}^M u_k^* y_k g(\mathbf{x}_k, \mathbf{x})\right)$$

#### Possible Kernels for Kernel Trick

Linear Kernel:  $g_{lin}(\mathbf{x}, \mathbf{x}_k) = \mathbf{x}_k^T \mathbf{x}$

Polynomial Kernel:  $g_{poly}(\mathbf{x}, \mathbf{x}_k) = (\mathbf{x}_k^T \mathbf{x} + 1)^d$

Sigmoid Kernel:  $g_{sigm}(\mathbf{x}, \mathbf{x}_k) = \tanh(\beta(\mathbf{x}_k^T \mathbf{x}) + w_0)$

Radial Kernel:  $g_{rbf}(\mathbf{x}, \mathbf{x}_k) = \exp(-\frac{1}{2\sigma^2} \|\mathbf{x} - \mathbf{x}_k\|_2^2)$

Support Vector Machine Representation.

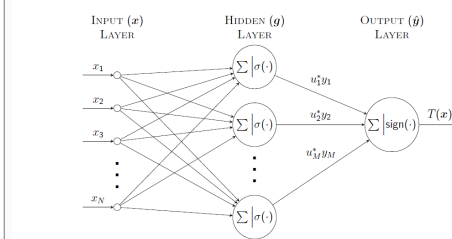


Fig. 2.4: The interpretation of a SUPPORT VECTOR MACHINE as a NEURAL NETWORK with three layers and a non-linear function  $\sigma$ . For POLYNOMIAL KERNELS each SINGLE HIDDEN LAYER UNIT is described by  $g_{pol}(\mathbf{x}, \mathbf{x}_k) = \sigma(z_k)$ , with  $\sigma(z_k) = z_k^d$  and  $z_k = \mathbf{x}_k^T \mathbf{x} + 1$ .

## 9. Learning and Generalization

#### 9.1. Empirical Risk Function and Generalization Error

ML scenarios (unknown Stochastical Model) base learning on:  $Risk_{emp}(T; \mathbb{S}) = \frac{1}{M} \sum_{i=1}^M L(T(\mathbf{x}_i), y_i), \quad (\mathbf{x}_i, y_i) \in \mathbb{S}$

$$\mathbf{x} \mapsto T(\mathbf{x}; \mathbb{S}) \quad T = \text{argmin}_{T' \in \mathbb{T}} \{Risk_{emp}(T'; \mathbb{S})\}$$

**good Generalization:**  $Risk_{emp}(T; \mathbb{S}_{test})$  similar to  $Risk_{emp}(T; \mathbb{S})$   
**bad Generalization:**

- small  $\mathbb{T}$  that does not cover  $T_{opt} \rightarrow$  cannot be selected by ML  $\Rightarrow$  strong mismatch between the desired and derived *Test* and refers to a sort of *Bias Error Term*
- too rich  $\mathbb{T} \rightarrow$  fluctuating of the available data (measurement noise) is interpreted as meaningful information  $\Rightarrow$  *Overfitting*; leads to an increased *Variance Error Term*

#### 9.2. Bias-Variance Decomposition

$$Risk = E_{S, X, Y} [L(T(X; S), Y)] = E_X [1 - P_{Y|X}(Y = T_B(X)) + (1 - P_{S|X}(T(X; S) = T_B(X))) (2P_{Y|X}(Y = T_B(X)) - 1)]$$

If the potential set  $\mathbb{S}$  would be selected from a distribution such that the derived Test  $T(\mathbf{x}; \mathbb{S})$  and the corresponding Bayes Test  $T_B(\mathbf{x})$  are identical almost surely, then the Risk Function achieves its minimum value which is equal to the *Irreducible Error*  $E_X [1 - P_{Y|X}(Y = T_B(X))]$  (denotes the probability that for a given input  $\mathbf{x}$  the Bayes Test  $T_B(X)$  decides for the false label  $y$ ).

## 10. Classification Trees and Random Forests

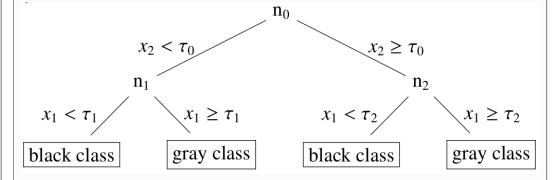
#### 10.1. CART Algorithms

Generate Binary Trees by splitting  $\mathbb{X}$  at each (internal/root) node:  $\mathbb{X}_{i, left} = \{\mathbf{x} \in \mathbb{X}_i | x_{j_i} < \tau_i\}$ ,  $\mathbb{X}_{i, right} = \mathbb{X}_i \setminus \mathbb{X}_{i, left}$

**Root/Internal node:** Binary decision based on chosen threshold  $\tau_i \in \mathbb{R}$ , feature  $x_{j_i} = \lfloor \mathbf{x} \rfloor_{j_i}$  with  $j_i \in \mathbb{J} = \{1, \dots, \dim[\mathbb{X}]\}$  aims at minimizing  $Risk_{emp}(T_{CART})$

**Terminal node:**  $n_i$  corresponds to subset  $\mathbb{X}_i \in \mathbb{X} \rightarrow$  has no more children; outputs a decision  $\Rightarrow \mathbf{x} \mapsto n_i(\mathbf{x})$

Example:



**Empirical Impurity Measure:** choose  $j_i$  and  $\tau_i$  at  $n_i$  by:  
 $I_{CART}(\mathbb{S}_i) = \sum_{k=1}^K (1 - \hat{P}_{Y|X}(Y = \theta_k | \{\mathbf{x} \in \mathbb{X}_i\}; \mathbb{S}_i)) \hat{P}_{Y|X}(Y = \theta_k | \{\mathbf{x} \in \mathbb{X}_i\}; \mathbb{S}_i)$   
with  
 $\hat{P}_{Y|X}(Y = \theta_k | \{\mathbf{x} \in \mathbb{X}_i\}; \mathbb{S}_i) = \frac{M_k(\mathbb{S}_i)}{M(\mathbb{S}_i)} = \frac{|\{(\mathbf{x}, y) \in \mathbb{S}_i | y = \theta_k\}|}{|\mathbb{S}_i|}$   
 $\Rightarrow \{j_i, \tau_i\} = \underset{j \in \mathbb{J}, \tau \in \mathbb{R}}{\operatorname{argmin}} \left\{ \sum_{k=1}^K \left( 1 - \frac{M_k(\mathbb{S}_i, left)}{M(\mathbb{S}_i, left)} \right) \frac{M_k(\mathbb{S}_i, left)}{M(\mathbb{S}_i)} + \left( 1 - \frac{M_k(\mathbb{S}_i, right)}{M(\mathbb{S}_i, right)} \right) \frac{M_k(\mathbb{S}_i, right)}{M(\mathbb{S}_i)} \right\}$   
**Overfitting** (comes with high purity) can be controlled by a **Test Set**  $\mathbb{S}_{Test}$ .  
**Decision Rule:** At terminal node  $n_i$ , input  $\mathbf{x}$  is assigned to  $T_{CART}(\mathbf{x}; \mathbb{S}) : \mathbb{X} \mapsto \{1, \dots, K\}, \mathbf{x} \mapsto \underset{k}{\operatorname{argmax}} \{M_k(\mathbb{S}_i)\}$

**Gini Impurity Index:**  $I_{CART} = \sum_{k=1}^K (1 - P_{Y|X}(\underline{y} = \theta_k | \{\mathbf{x} \in \mathbb{X}\})) P_{Y|X}(\underline{y} = \theta_k | \{\mathbf{x} \in \mathbb{X}\}) = \sum_{k=1}^K \sum_{j=1, j \neq k}^K P_{Y|X}(\underline{y} = \theta_j | \{\mathbf{x} \in \mathbb{X}\}) P_{Y|X}(\underline{y} = \theta_k | \{\mathbf{x} \in \mathbb{X}\})$

## 10.2. Random Forests

Avoid **Overfitting** (here: CART)  $\Rightarrow$  combine independent *Hypothesis Tests*: e.g. by **Majority Vote**  
 $T_{maj}(\mathbf{x}) = \underset{t=1}{\operatorname{majority}} \{T_{CART}(\mathbf{x}; \mathbb{S}^{(t)}, \nu^{(t)})\}_{t=1}^{t_{max}}$   
**Randomization Parameter**  $\nu_i$  controls an additionally introduced Randomness between the individual Tests.  
 $\Rightarrow$  **Variance** of  $T_{avg}(\mathbf{x})$  is reduced by  $1/t_{max}$  with respect to the **Variance** of the individual test.

**Random Forest Method:**

- $T_{RF}(\mathbf{x}) = \underset{t=1}{\operatorname{majority}} \{T_{CART}(\mathbf{x}; \mathbb{S}^{(t)}, \mathbb{J}^{(t)})\}_{t=1}^{t_{max}}$
- Stochastic Independence by Bootstrapping of training samples (random sampling from  $\mathbb{S}$  with replacement)  $\Rightarrow$  large  $t_{max}$  guarantees excellent performance (yet Tests are still correlated)
- Overfitting not considered (maximum purity)  $\Rightarrow$  small bias of RF Method

## 10.3. From Kernel to Neural Networks (NN)

NN: methodology by which KERNELS are determined by chosen learning method based on the available training data  $\rightarrow$  KERNELS are composed by a concatenation of multiple VECTOR VALUED functions

$$g(x) = f^{(L)}(f^{(L-1)}(\dots f^{(2)}(f^{(1)}(x; W^{(1)}, v^{(1)}); W^{(2)}, v^{(2)}) \dots; W^{(L-1)}, v^{(L-1)}); W^{(L)}, v^{(L)})$$

$f^{(l)}(*; W^{(l)}, v^{(l)}) \in \mathbb{R}^{N_l}$  represents the  $l$ -th layer of NN  
NN consist of  $L+2$  layers (INPUT Layer  $x \in \mathbb{R}^N$  and LAYER OF OUTPUTS  $f^{(NN)} \in \mathbb{R}^{N_{L+1}}$   
HIDDEN LAYER ( $L=1$ ) often enough  
If  $L > 1$  NN is called **DEEP**

Mapping between NN layers consists typically of AFFINE TRANSFORMATION of the output of the preceding layer;  
 $\mathbb{R}^{N_{l-1}} \rightarrow \mathbb{R}^{N_l} : f^{(l-1)} \rightarrow (l) = W^{(l),T} f^{(l-1)} + v^{(l)}$ ,  
and the elementwise **NONLINEAR TRANSFORMATION** of the resulting INTERNAL STATE VECTOR  $z^{(l)}$  by means of a **NONLINEAR FUNCTION**  $\sigma^{(l)}$

$$f^{(l)}(f^{(l-1)}; W^{(l)}, v^{(l)}) = \sigma^{(l)}(W^{(l),T} f^{(l-1)} + v^{(l)})$$

Elements of  $^{(l)}$  and  $v^{(l)}$  are called weights of the  $l$ th NN layer

- INPUT LAYER ( $l=0$ ) of NN equals INPUT VECTOR  $x \in \mathbb{R}^N$
- OUTPUT LAYER ( $l=L+1$ ) of NN equals OUTPUT VECTOR  $f^{(NN)} \in \mathbb{R}^{N_{L+1}}$
- **NONLINEAR FUNCTION**  $\sigma_i^{(l)}$  of the HIDDEN LAYERS is different from the OUTPUT FUNCTION of the OUTPUT LAYER
- latter depends on LOSS FUNCTION and the chosen LEARNING ALGORITHM

Single nonlinear function of the output vector of the previous layer composed by the  $i$ -th LINEAR FUNCTIONAL  $w_i^{(l)}$ , the CONSTANT  $v_i^{(l)}$  and the  $i$ -th nonlinear function  $\sigma^{(l)}$  of the next layer = NEURON. WEIGHTS represent the SYNAPTIC STRENGTHS and the nonlinear function  $\sigma_i^{(l)}$  = ACTIVATION FUNCTION

$$\sigma_i^{(l)}(\sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} f_j^{(l-1)} + v_i^{(l)})$$

**Signal Neuron:**

Single Neuron Representation.

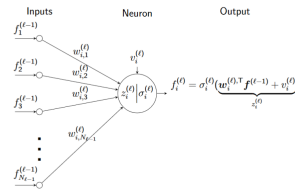


Fig. 5.1: A single neuron representation of the  $i$ -th output element of the  $l$ -th network layer

**Neural Network:**  
**Neural Network.**

Representation of a FEEDFORWARD NEURAL NETWORK – aka MULTILAYER PERCEPTRON (MLP)

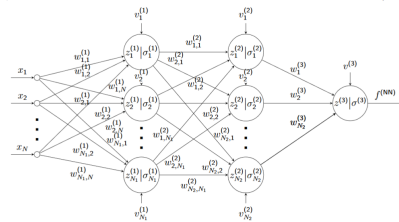


Fig. 5.2: DEEP NN with an input layer, two hidden layers, and one output function.

## 10.4. Activation Functions

**ReLU Activation Functions**

most popular chose for the activation function  $\sigma_i^{(l)} \rightarrow$  RECTIFIED LINEAR UNIT FUNCTION (RELU)

$$\sigma(z_i^{(l)}) = \max(0, z_i^{(l)}) \in \mathbb{R}_+$$

with  $z_i^{(l)} = \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} f_j^{(l-1)} + v_i^{(l)}$

- PIECEWISE LINEAR FUNCTION which is zero for a negative state variable
- efficient for the training of network weights, since its gradient with respect to the weight parameters does not experience any saturation for large positive values of the state variable, i.e.

$$\frac{\partial \sigma(z_i^{(l)})}{\partial w_{i,j}^{(l)}} = \frac{\partial \sigma(z_i^{(l)})}{\partial z_i^{(l)}} \frac{\partial z_i^{(l)}}{\partial w_{i,j}^{(l)}} = \text{unit}(z_i^{(l)} f_j^{(l-1)}) \text{ and } \frac{\partial \sigma(z_i^{(l)})}{\partial v_{i,j}^{(l)}} = \frac{\partial \sigma(z_i^{(l)})}{\partial z_i^{(l)}} \frac{\partial z_i^{(l)}}{\partial v_{i,j}^{(l)}} = \text{unit}(z_i^{(l)})$$

with the UNIT STEP FUNCTION  $\text{unit}(z) \in \{0, 1\}$

RELU AF:

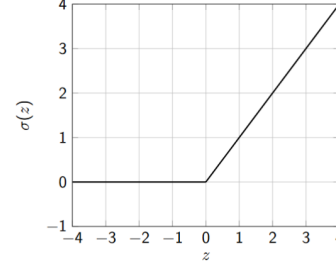


Fig. 5.3: The ReLU activation function  $\sigma(z) = \max\{0, z\}$ .

**Hyperbolic Tangent Activation Functions**

Used to be standard before RELU

$$\sigma(z_i^{(l)}) = \tanh(z_i^{(l)}) = \frac{e^{z_i^{(l)}} - e^{-z_i^{(l)}}}{e^{z_i^{(l)}} + e^{-z_i^{(l)}}} \in [-1, +1]$$

with  $z_i^{(l)} = \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} f_j^{(l-1)} + v_i^{(l)}$

The **HYPERBOLIC TANGENT FUNCTION** suffers from a saturation of its gradient with respect to weight parameters for large absolute values of the state variable, i.e.

$$\frac{\partial \omega(z_i^{(l)})}{\partial w_{i,j}^{(l)}} = \frac{\partial \omega(z_i^{(l)})}{\partial z_i^{(l)}} \frac{\partial z_i^{(l)}}{\partial w_{i,j}^{(l)}} = (1 - \tanh^2(z_i^{(l)})) f_j^{(l-1)} \text{ and } \frac{\partial \omega(z_i^{(l)})}{\partial v_i^{(l)}} = (1 - \tanh^2(z_i^{(l)}))$$

Advantage: for small values of the state variable near  $z_i^{(l)} = 0$  the **HYPERBOLIC TANGENT FUNCTION** resembles a **LINEAR MODEL**

**HYPERBOLIC TANGENT FUNCTION** is very similar to s.c. **SIGMOID FUNCTION**  $\omega_{SIGMOID}(z_i^{(l)}) = \frac{1}{1 + e^{-z_i^{(l)}}}$

$$\rightarrow \tanh(z_i^{(l)}) = 2\sigma_{SIGMOID}(2z_i^{(l)}) - 1$$

**Hyperbolic Tangent AF:**

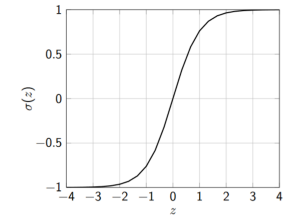


Fig. 5.4: The **HYPERBOLIC TANGENT** activation function  $\sigma(z) = \tanh(z)$   
**Sigmoid AF:**

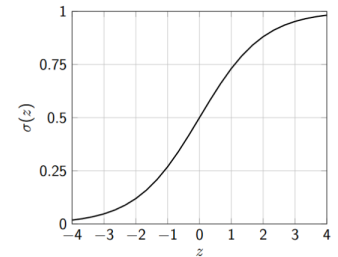


Fig. 5.5: The **SIGMOID** activation function  $\sigma(z) = (1 + e^{-z})^{-1}$