# Rules of Probability

Sum Rule: $p(X) = \sum_Y p(X, Y)$

Product Rule: $p(X, Y) = p(Y|X) \cdot p(X)$

Bayes' Theorem: $p(Y|X) = \frac{p(X, Y)}{p(X)}$ where

$p(X) = \sum_Y p(X|Y) p(Y)$

Conditional Expectation: $E_x[f|y] = \sum_x p(x|y) f(x)$

# Bayes Decision Theory

1. **Priors**: $p(C_k)$ — A priori — what we can tell about the probability before seeing the data

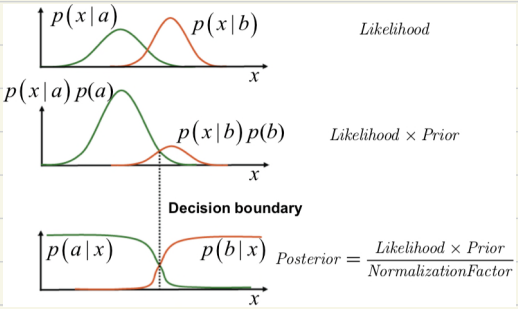
2. **Conditional probabilities**: $p(x|C_k)$ — Likelihood for class $C_k$

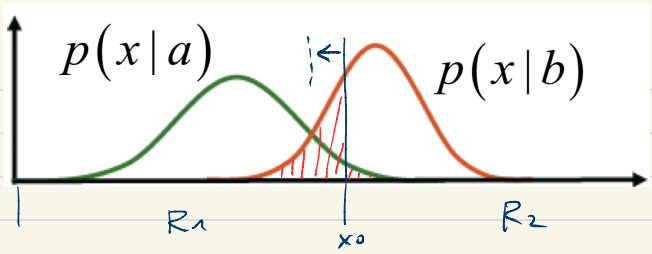
   $x$: feature vector

3. **Posterior** $p(C_k|x)$: the probability of $C_k$ given the $x$.

$$p(C_k|x) = \frac{p(x|C_k) \cdot p(C_k)}{p(x)} = \frac{p(x|C_k) \cdot p(C_k)}{\sum_i p(x|C_i) \cdot p(C_i)}$$

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{Normalisation Factor}}$$






$p(\text{mistake}) = p(x \in R_1, b) + p(x \in R_2, a)$

$=$ Area

Move $k_0 \rightarrow$ to the optimised

Optimal decision rule: $p(C_1|x) > p(C_2|x)$

$\Leftrightarrow \quad \frac{p(x|C_1)}{p(x|C_2)} > \frac{p(C_2)}{p(C_1)} = \theta$ (decision threshold)

[Likelihood ratio test]

Minimise the expected loss: $E[L] = \sum_k \sum_j \int_{R_j} L_{kj}\, p(x, C_k)\, dx$

$\sim = \sum_k L_{kj}\, p(C_k|x)$

posterior

Risk $\begin{cases} R(\alpha_1|x) = L_{11}\, p(C_1|x) + L_{21}\, p(C_2|x) \\ R(\alpha_2|x) = L_{12}\, p(C_1|x) + L_{22}\, p(C_2|x) \end{cases}$

$R(\alpha_2|x) > R(\alpha_1|x) \quad \Leftrightarrow \quad \frac{p(x|C_1)}{p(x|C_2)} > \frac{(L_{21} - L_{22})\, p(C_2)}{(L_{12} - L_{11})\, p(C_1)}$

Reject Option: the largest posterior probability $p(C_k|x)$ is significantly less than 1.

## Discriminant Function

- $y_k(x) \propto p(x|C_k) \cdot p(C_k)$ : Generative Methods
  First determin the class-conditional densities for each class individually and separately infer the prior class probabilities. Then use Bayes' Theorem to determine class.
- $y_k(x) = p(C_k|x)$ : Discriminative Methods
  First solve the inference problem of determining the posterior class prob.
  Then use decision theory to assign each new $x$ to its class.

To solve : $x \rightarrow C_k$ : $p(C_k|x)$

posterior

- Parametric Representation
- Non-Parametric Representation
- Mixture Models.

**Gaussian**

$$N(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

$$N(x|\mu,\Sigma) = \frac{1}{(2\pi)^{D/2}\,|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right\}$$

$\Delta^2 = (x-\mu)^T\Sigma^{-1}(x-\mu)$ : $\Delta$ : Mahalanobis Distance.

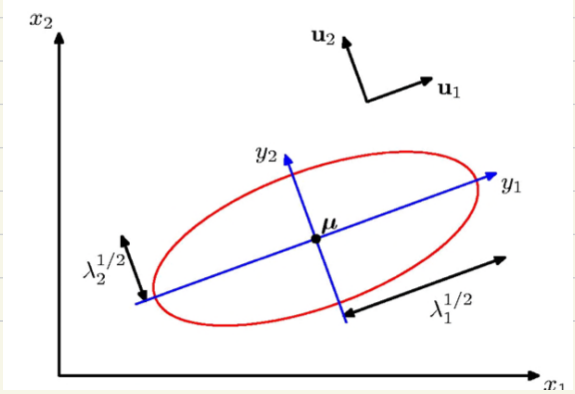
$$\Sigma = \sum_{i=1}^{D} \lambda_i u_i u_i^T \quad , \quad \Sigma^{-1} = \sum_{i=1}^{D} \frac{1}{\lambda_i} u_i u_i^T$$

$$\Rightarrow \Delta^2 = \sum_{i=1}^{D} \frac{y_i^2}{\lambda_i^2} \quad \text{with} \quad y_i = u_i^T(x-\mu)$$

$$= \sum_{i=1}^{D} \frac{(u_i^T(x-\mu))^T \cdot (u_i^T(x-\mu))}{\lambda_i^2} = \sum_{i=1}^{D} \frac{(x-\mu)^T u_i u_i^T (x-\mu)}{\lambda_i^2} = (x-\mu)^T \cdot \Sigma^{-1} \cdot (x-\mu)$$

$\rightsquigarrow$ Contant density on ellipsoids with main directions along the eigenvectors $u_i$ and scaling factors $\sqrt{\lambda_i}$

$\Sigma$ diag : Axis-aligned / $\Sigma = \sigma^2 I$ : Hypersphere.



# Parametric Methods

$L(X|\theta)$ : Likelihood of $\theta$ : Probability that $X$ have indeed been generated from pd with $\theta$.

**ML Estimation**: $E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$

(1D) $E(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\mu,\sigma)$

$$= -\sum_{n=1}^{N} \ln\left(\frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{\|x_n-\mu\|^2}{2\sigma^2}\right\}\right)$$

$$\frac{\partial E(\theta)}{\partial \mu} = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \mu} p(x_n|\mu,\sigma)}{p(x_n|\mu,\sigma)} = -\sum_{n=1}^{N} \frac{2(x_n-\mu)}{2\sigma^2}$$

$$= \frac{1}{\sigma^2}\sum_{n=1}^{N}(x_n-\mu) \stackrel{!}{=} 0 \quad \Rightarrow \quad \hat{\mu} = \frac{1}{N}\sum_{n=1}^{N} x_n \quad / \hat{\sigma}^2 = \frac{1}{N}\sum_{n=1}^{N}(x_n-\hat{\mu})^2$$

Biased ! To fix : $\tilde{\sigma}^2 = \frac{N}{N-1}\sigma_{ML}^2 = \frac{1}{N-1}\sum_{n=1}^{N}(x_n-\hat{\mu})^2$

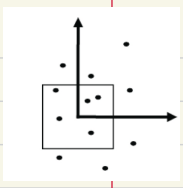
Limitations :
- It systematically underestimates $\sigma$ of distribution.
- Overfits to the observed data.

## Non-Parametric Methods : Estimate probability density

**Histogram** $p_i = \frac{n_i}{N \cdot \Delta_i}$

- General : In the limit $N \to \infty$ every pd can be represented
- No need to store data once hist is compu
- Rather brute-force

- Curse of dimensionality : D / M bins/d : $M^D$ bins (exponential)
- Discontinuities at bin edges.
- Bin size ?
  - too large : too much smoothing
  - too small : too much noise



$$p(x) \approx \frac{K}{NV}$$

{ local region sufficiently small.
$p(x)$ in $R$ roughly constant
$N$ sufficiently large

fixed $V$, determine $K$: Kernel Methods

fixed $K$, determine $V$: KNN

**Parzen Window**

$$k(u) = \begin{cases} 1, & |u_i| \le \frac{1}{2}h \\ 0, & \text{else.} \end{cases}$$

$$K = \sum_{n=1}^{N} k(x - x_n) \quad , \quad V = \int k(u)\,du = h^D$$

$$p(x) = \frac{K}{NV} = \frac{1}{Nh^D} \sum_{n=1}^{N} k(x - x_n)$$

**Gaussian Kernel**

$$k(u) = \frac{1}{(2\pi h^2)^{1/2}} \exp\left\{-\frac{u^2}{2h^2}\right\}$$

$$K = \sum_{n=1}^{N} k(x - x_n) \quad , \quad V = \int k(u)\,du = 1$$

$$p(x) \approx \frac{K}{NV} = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi)^{D/2} h} \cdot \exp\left\{-\frac{\|x - x_n\|^2}{2h^2}\right\}$$

In general: $k(u) \ge 0$, $\int k(u)\,du = 1$,

$$K = \sum_{n=1}^{N} k(x - x_n) \quad , \quad p(x) \approx \frac{K}{NV} = \frac{1}{N} \sum_{n=1}^{N} k(x - x_n)$$

Kernel / KNN:

- General. In the limit $N \to \infty$, every probability density can be represented.
- No computation involved in the training phase. (simply storage)
- Requires storing & computing with entire dataset.
- computational cost: linear → # data (~> Tree)

$h$ / $K$ { too large → too smooth
too small → not smooth enough.

# MoG

$$p(x|\theta) = p(x|\theta_j)\, p(j)$$

prior of component $j$

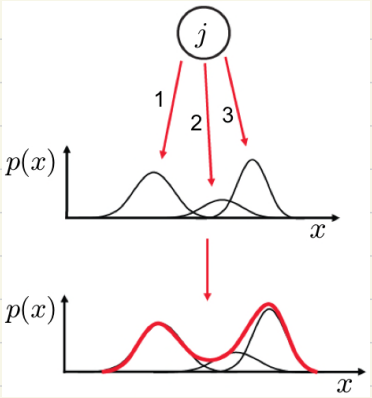
$p(j) = \pi_j$ with $\pi_j \in (0,1)$ & $\sum_{j=1}^{M} \pi_j = 1$

$$p(x|\theta_j) = \mathcal{N}(x|\mu_j, \sigma_j^2) = \frac{1}{\sqrt{2\pi}\sigma_j} \cdot \exp\left\{-\frac{1}{2\sigma_j^2}(x-\mu_j)^2\right\}$$

likelihood of $x$ given mixture component $j$

Note: · $\int p(x)\,dx = 1$.

· Mixture parameter: $\theta = (\pi_1, \mu_1, \sigma_1, \dots, \pi_M, \mu_M, \sigma_M)$




Generative model:

$$p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j)\, p(j)$$

Mixture density — Weight of mixture component — Mixture component

## Estimation Attempt:

Minimize $E = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$

with $\ln p(X|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k) \right\}$

$$\frac{\partial E}{\partial \mu_j} = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \mu_j} p(x_n|\theta_j)}{\sum_{k=1}^{K} p(x_n|\theta_k)} = -\sum_{n=1}^{N} \left( \Sigma^{-1}(x_n - \mu_j) \frac{p(x_n|\theta_j)}{\sum_{k=1}^{K} p(x_n|\theta_k)} \right)$$

$$\frac{\partial}{\partial \mu_j} \mathcal{N}(x_n|\mu_k, \Sigma_k) = \Sigma^{-1}(x_n - \mu_j)\, \mathcal{N}(x_n|\mu_k, \Sigma_k)$$

$$= -\Sigma^{-1} \sum_{n=1}^{N} (x_n - \mu_j) \cdot \frac{\pi_j \mathcal{N}(x_n|\mu_j, \Sigma_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)} \stackrel{!}{=} 0$$

$:= \gamma_j(x_n)$ responsibility

$$\Rightarrow \sum_{n=1}^{N} (x_n - \mu_j) \cdot \gamma_j(x_n) = 0, \quad \mu_j = \frac{\sum_{n=1}^{N} \gamma_j(x_n) \cdot x_n}{\sum_{n=1}^{N} \gamma_j(x_n)}$$

↓

No direct analytical solution !

# EM ( Expectation Maximization )

## K-Means – Clustering:

- Initialisation: pick K arbitary centroids ( cluster means)

E → • Assign each sample to the closest centroid

M → • Adjust the centroids to be the means of the samples assigned to

• Goto , until no change.

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \| x_n - \mu_k \|^2$$

where $r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \| x_n - \mu_j \|^2 \\ 0 & \text{otherwise} \end{cases}$

( Indicator to check whether $\mu_k$ is the nearest cluster center to point $x_n$ )

\+ Simple, fast to compute.

\+ Converges to local optimum of within-cluster squared error

\- Setting k ?

\- sensitive to initial centers

\- Sensitive to outliers

\- Detects spherical clusters only

→ Speedups through search structures

→ K-Medoids ( member of data).

## Credit Assignment Problem

$$p(j=1 \mid x, \theta) = \frac{p(j=1, x \mid \theta)}{p(x \mid \theta)}$$

Evaluate posterior probability that an observed x was generated from 1. Mixture component.

$$p(j=1, x \mid \theta) = p(x \mid j=1, \theta)\, p(j=1) = p(x \mid \theta_1)\, p(j=1)$$

$$p(j=1 \mid x, \theta) = \frac{p(x \mid \theta_1)\, p(j=1)}{\sum_{j=1}^{2} p(x \mid \theta_j)\, p(j)} = \gamma_j(x)$$

**E-Step:** softly assign samples to mixture components.

$$\gamma_j(x_n) \leftarrow \frac{\pi_j \mathcal{N}(x_n | \mu_j, \Sigma_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k)} \quad , \forall j = 1 \cdots K, \; n = 1 \cdots N$$

**M-Step:** re-estimate the parameters (separately for each mixture component) based on the soft assignments.

$$\hat{N}_j \leftarrow \sum_{n=1}^{N} \gamma_j(x_n) \quad = \text{soft number of samples labeled } j$$

$$\hat{\pi}_j^{new} \leftarrow \frac{\hat{N}_j}{N}, \quad \hat{\mu}_j^{new} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(x_n) \cdot x_n$$

$$\hat{\Sigma}_j^{new} \leftarrow \frac{1}{\hat{N}} \sum_{n=1}^{N} r_j(x_n)(x_n - \hat{\mu}_j^{new})(x_n - \hat{\mu}_j^{new})^T$$

**Techniques:**

- use $(\Sigma + \sigma_{min} I)^{-1}$ instead of $\Sigma^{-1}$ to avoid singularity
- Initialise with K-Means!
  (Arbitary, but convergence much faster)
- – Run kMeans M times (10~100)
  – Pick the best result (lowest J)
  – Use it as initial:
    - Set $\mu_j$ to the corresponding cluster mean from k-Means
    - Initialise $\Sigma_j$ to the sample covariance of the associated data.

## MoG Summary:

+ General, can represent any continuous distribution.
+ Once trained, fast to evaluate
+ Can be updated online.
- Avoid singularity
– Computationally expensive (high dim. More overhead & slow converge vs. K Mea
  Sensitive to initial.
– Select K.

# Discriminant Function

Bayesian:
- Model conditional pd: $p(x|C_k)$
  prior prob: $p(C_k)$
- Compute $p(C_k|x)$
- Min. Misclassification by max. $p(C|x)$

New:
- Directly encode decision boundary
- Without explicit modeling of pd.
- Minimise misclass prob. directly.

Linear discriminant function: $y(x) = w^T x + w_0$

$w$: weight vec; $w_0$: bias, threshold

$$\boxed{y(x) = \tilde{w}^T \tilde{x}}$$

$$= \sum_{i=0}^{D} w_i x_i \quad \text{with } x_0 = 1$$

To solve: $Y(\hat{X}) = \hat{X}\tilde{w}$, $\hat{X}\tilde{w} - T$ min

Least-Square: sum of square error

$$E(w) = \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} (y_k(x_n; w) - t_{kn})^2$$

$$= \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} (w_k^T x_n - t_{kn})^2$$

Matrix

$$E_D(\tilde{w}) = \frac{1}{2} Tr\{(\tilde{X}\tilde{w} - T)^T (\tilde{X}\tilde{w} - T)\}$$

$\sum_{ij} a_{ij}^2 = Tr(A^T A)$

$$\frac{\partial}{\partial \tilde{w}} E_D(\tilde{w}) = \frac{1}{2} \frac{\partial}{\partial \tilde{w}} Tr\{(\tilde{X}\tilde{w} - T)^T (\tilde{X}\tilde{w} - T)\}$$

$$= \frac{1}{2} \frac{\partial}{\partial (\hat{X}\hat{w} - T)^T (\hat{X}\hat{w} - T)} Tr\{(\tilde{X}\tilde{w} - T)^T (\tilde{X}\tilde{w} - T)\} \cdot \frac{\partial}{\partial \tilde{w}} (\hat{X}\hat{w} - T)^T (\hat{X}\hat{w} - T)$$

$$= \tilde{X}^T (\tilde{X}\tilde{w} - T) \doteq 0$$

$\frac{\partial}{\partial A} Tr\{A\} = I$

$$\Rightarrow \tilde{w} = \tilde{X}^+ T, \quad y(x) = \tilde{w}^T \tilde{x} = T^T (\tilde{X}^+)^T \tilde{x}$$

- Least - Square: LS corresponds to ML under the assumption of Gaussian.

↝ Generalised linear Models

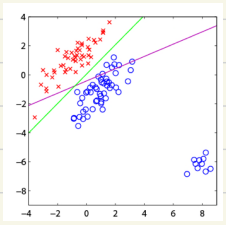
Activation function (monotonous ↗): $g(\cdot)$ : $y(x) = g(w^T x + w_0)$

$$p(C_1|x) = \frac{p(x|C_1)\,p(C_1)}{p(x|C_1)p(C_1) + p(x|C_2)\,p(C_2)} = \frac{1}{1 + \frac{p(x|C_2)p(C_2)}{p(x|C_1)p(C_1)}} = \frac{1}{1+e^{-a}}$$

Logistic Sigmoid: $g(a) \equiv \frac{1}{1+e^{-a}}$

Normalised Exponential / Softmax: ↝ perceptron

$$p(C_k|x) = \frac{p(x|C_k)\,p(C_k)}{\sum_j p(x|C_j)\,p(C_j)} = \frac{e^{a_k}}{\sum_j e^{a_j}}$$ ↝ posterior



Motivation of Nonlinearity
- limit the influences of "too correct" data points
- Not linear separable

Generalized Linear Models

+ Nonlinearity → more flexibility
+ to limit the effect of outliers
+ Choice of Sigmoid leads to a nice probabilistic interpretation
- Least Square Min. in general not analytically solved
⇒ iterative
⇒ Gradient Descent

## BasisFunction

$$y_k(x) = \sum_{j=1}^{M} w_{kj}\,\phi_j(x) + w_{k0} = \sum_{j=0}^{M} w_{kj}\,\phi_j(x) \quad \text{with } \phi_0(x) = 1$$

↳ basis function
- Allow non-linear decision boundaries
- By choosing the right $\phi_j$, every continuous func. can be approximated with arbitrary accuracy.

# Gradient Descent

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(w)}{\partial w_{kj}} \right|_{w^{(\tau)}}$$

Batch learning: Compute gradient based on all training data

$$\frac{\partial E(w)}{\partial w_{kj}}$$

Sequential updating: Compute grad based on a single data point at a time

$$\frac{\partial E_n(w)}{\partial w_{kj}}$$

Error Function: $E(w) = \sum_{n=1}^{N} E_n(w) = \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \left( \sum_{j=1}^{M} w_{kj} \phi_j(x_n) - t_{kn} \right)^2$

$$\Rightarrow E_n(w) = \frac{1}{2} \sum_{k=1}^{K} \left( \sum_{j=1}^{M} w_{kj} \phi_j(x_n) - t_{kn} \right)^2$$

$$\frac{\partial E_n(w)}{\partial w_{kj}} = \left( \sum_{j=1}^{M} w_{kj} \phi_j(x_n) - t_{kn} \right) \phi_j(x_n)$$

$$= (y_k(x_n; w) - t_{kn}) \phi_j(x_n)$$

Delta Rule: $w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta (y_k(x_n; w) - t_{kn}) \phi_j(x_n)$

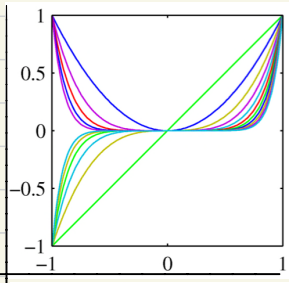
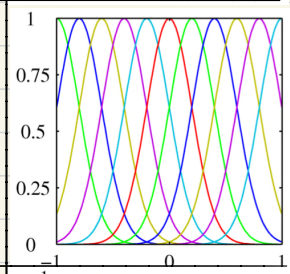
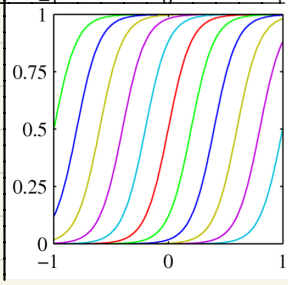
$$= w_{kj}^{(\tau)} - \eta \delta_{kn} \phi_j(x_n)$$

Activation function diff'bar, non linear: $\delta_{kn} = \frac{\partial g(a_k)}{\partial w_{kj}} (y_k(x_n; w) - t_{kn})$

$$y_k(x) = g(a_k) = g\left( \sum_{j=0}^{M} w_{ki} \phi_j(x_n) \right)$$

+ General class of decision function
+ $g(\cdot)$ + $\phi_j$ allow non-separable.
+ GD or 2. order GD (Newton–Raphson)
- curse of dim: $g(\cdot)$ + $\phi_j$ introduce additional para.
- Overfitting

# Linear basis function $\phi_j$

| | | |
|---|---|---|
| Polynomial<br>$\phi_j(x) = x^j$ | Global: A small change in x affects all basis functions.<br>The decision boundary: polynomial func of x (Non linear)<br>Still solve a linear problem in $\phi(x)$ |  |
| Gaussian<br>$\phi_j(x) = \exp\{-\frac{(x-\mu_j)^2}{2s^2}\}$ | Local: A small change in x affects only nearby basis functions<br>$\mu_j$ and s control location and scale (width) |  |
| Sigmoid<br>$\phi_j(x) = \sigma(\frac{x-\mu_j}{s})$<br>$\sigma(a) = \frac{1}{1+e^{-a}}$ | Local: A small change in x affects only nearby basis functions<br>$\mu_j$ and s control location and scale (slope) |  |

# Probabilistic Discriminative Models

$$p(C_1|x) = \sigma(a) = \frac{1}{1+e^{-a}}, \quad a = \ln\frac{p(x|C_1)p(C_1)}{p(x|C_2)p(C_2)}, \quad a = w^T\phi(x)$$

## Logistic Regression

$$p(C_1|\phi) = y(\phi) = \sigma(w^T\phi)$$

$$p(C_2|\phi) = 1 - p(C_1|\phi)$$

$$p(C_1|\phi) = \frac{p(\phi|C_1)p(C_1)}{p(\phi|C_1)p(C_1) + p(\phi|C_2)p(C_2)}$$

# Parameter:

2 classes

M-dim $\phi$

Mean: $2M$ $\dim(\vec{\phi}_1) + \dim(\vec{\phi}_2)$

Covariance: $\frac{M\cdot(M+1)}{2}$ $\text{cov}(\Delta)$

Class: 1

$$\Big\} \quad \frac{M(M+5)}{2} + 1$$

$$p(C_1|\phi) = y(\phi) = \sigma(w^T\phi) \quad : \quad M$$

Logistic Sigmoid $\sigma(a) = \frac{1}{1+e^{-a}}$, $\rightsquigarrow a = \ln\left(\frac{\sigma}{1-\sigma}\right)$

Symmetry: $\sigma(-a) = 1 - \sigma(a)$

Derivative: $\frac{d\sigma}{da} = \sigma(1-\sigma)$

With $y_n = p(C_1|\phi_n)$: $p(t|w) = \prod_{n=1}^{N} y_n^{t_n}\{1-y_n\}^{1-t_n}$ (Likelihood)

Negative Log-likelihood $E(w) = -\ln p(t|w)$

Cross-Entropy $= -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$

$$\nabla E(w) = -\sum_{n=1}^{N}\left\{t_n \frac{\frac{d}{dw}y_n}{y_n} + (1-t_n)\frac{\frac{d}{dw}(1-y_n)}{1-y_n}\right\}$$

$y_n = \sigma(w^T\phi_n)$

$\frac{d}{dw}y_n = y_n(1-y_n)\phi_n$

$$= -\sum_{n=1}^{N}\left\{t_n \frac{y_n(1-y_n)}{y_n}\phi_n - (1-t_n)\frac{y_n(1-y_n)}{1-y_n}\phi_n\right\}$$

$$\sim = \sum_{n=1}^{N}(y_n - t_n)\phi_n$$

Delta Rule: $w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta\,(y_k(x_n;w) - t_{kn})\,\phi_j(x_n)$

⇒ A more efficient iterative method:

## 2. order Newton-Raphson Gradient descent:

$w^{(\tau+1)} = w^{(\tau)} - H^{-1}\nabla E(w)$ with $H = \nabla\nabla E(w)$ (Hessian)

- Local quadratic approximation to the log-likelihood.
- Faster convergence

## Newton-Raphson for LSE (Least-Squares Estimation)

$$E(w) = \frac{1}{2}\sum_{n=1}^{N}(w^T\phi_n - t_n)^2$$

$$\nabla E(w) = \sum_{n=1}^{N}(w^T\phi_n - t_n)\phi_n = \Phi^T\Phi w - \Phi^T t$$

$$\Phi = \begin{bmatrix} \phi_1^T \\ \vdots \\ \phi_N^T \end{bmatrix}$$

$$\nabla\nabla E(w) = \sum_{n=1}^{N}\phi_n\phi_n^T = \Phi^T\Phi$$

$$\Rightarrow w^{(\tau+1)} = w^{(\tau)} - (\Phi^T\Phi)^{-1}(\Phi^T\Phi w^{(\tau)} - \Phi^T t)$$

$$= (\Phi^T\Phi)^{-1}\Phi^T t \qquad \text{Closed-form !}$$

## Newton-Raphson for cross-entropy:

$$E(w) = -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$

$$\nabla E(w) = \sum_{n=1}^{N}(y_n - t_n)\phi_n = \Phi^T(y-t)$$

$$\frac{dy_n}{dw} = y_n(1-y_n)\phi_n$$

$$\nabla\nabla E(w) = \sum_{n=1}^{N} y_n(1-y_n)\phi_n\phi_n^T = \Phi^T R\Phi$$

↑ weighting Matrix

$R_{nn} = y_n(1-y_n)$.
$R$ : diagonal

$$\Rightarrow w^{(\tau+1)} = w^{(\tau)} - (\Phi^T R\Phi)^{-1}\Phi^T(y-t)$$

$$= (\Phi^T R\Phi)^{-1}\cdot(\Phi^T R\Phi w^{(\tau)} - \Phi^T(y-t))$$

$$= (\Phi^T R\Phi)^{-1}\Phi^T R z$$

with $z = \Phi w^{(\tau)} - R^{-1}(y-t)$

- $R$ non-constant (depends on $w$)
- Need to apply normal equations iteratively

⇝ *Iteratively Reweighted Least-Squares*

**Logistic Regression Summary**

- Directly represent posterior $p(\phi|C_k)$
- Fewer para than likelihood+prior
- Cross-entropy is concave: Unique optim., no closed-form, IRLS
- Both online & Batch optimisations exist.
- Tend to systematically overestimate odds ratios when sample size $< \sim 500$.

# Softmax Regression

– Multiclass generalisation of logistic regression:

In logistic regression : $t_n \in \{0, 1\}$

Softmax : K values in 1-of-K notation

$$y(x; w) = \begin{bmatrix} P(y=1 \mid x; w) \\ P(y=2 \mid x; w) \\ \vdots \\ P(y=K \mid x; w) \end{bmatrix} = \frac{1}{\sum_{j=1}^{K} \exp(w_j^T x)} \cdot \begin{bmatrix} \exp(w_1^T x) \\ \exp(w_2^T x) \\ \vdots \\ \exp(w_K^T x) \end{bmatrix}$$

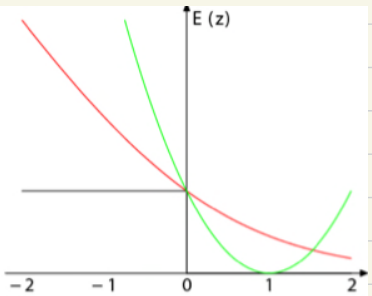
$$\sim \frac{\exp(a_K)}{\sum \exp(a_K)} \qquad \text{(normalised)}$$

Logistic : $$E(w) = -\sum_{n=1}^{N} \sum_{k=0}^{1} \{ \mathbb{I}(t_n = k) \ln P(y_n = k \mid x_n; w) \}$$

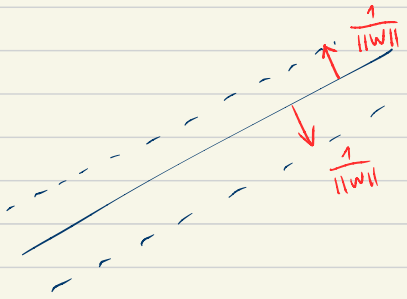
Softmax : $$E(w) = -\sum_{n=1}^{N} \sum_{k=1}^{K} \left\{ \mathbb{I}(t_n = k) \ln \frac{\exp(w_k^T x)}{\sum_{j=1}^{K} \exp(w_j^T x)} \right\}$$

GD : $$\nabla_{w_K} E(w) = -\sum_{n=1}^{N} [ \mathbb{I}(t_n = k) \ln P(y_n = k \mid x_n; w) ]$$

- Ideal Misclassification Error
  - This is what we would like to optimize.
  - But cannot compute gradients here.
- Quadratic Error
  - Easy to optimize, closed-form solutions exist.
  - But not robust to outliers.
- Cross-Entropy Error
  - Minimizer of this error is given by posterior class probabilities.
  - Concave error function, unique minimum exists.
  - But no closed-form solution, requires iterative estimation.



# SVM




$t_n(w^T x_n + b) \geq 1 \quad \forall n$

maximising margin $\Leftrightarrow$ $\min \|w\|^2$

Original QP : $\underset{w,b}{\operatorname{argmin}} \frac{1}{2}\|w\|^2$ , s.t. $t_n(w^T x_n + b) \geq 1 \quad \forall n$

SGD

Primal : $L_p = \frac{1}{2}\|w\|^2 - \sum_{n=1}^{N} a_n (t_n y(x_n) - 1)$

KKT : $a_n \geq 0$ , $t_n y(x_n) - 1 \geq 0$ , $a_n(t_n y(x_n) - 1) = 0$

KKT:
$\lambda \geq 0$
$f(x) \geq 0$
$\lambda f(x) = 0$

$d+1$ variables

Dual : $L_d(a) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m K(x_m, x_n)$

$0 \leq a_n \leq C$

$\sum_{n=1}^{N} a_n t_n = 0$

$w = \sum_{n=1}^{N_s} a_n t_n x_n$ ← support vectors

$n+1$ variables

Comparison: Primal Dual

$L_d$ only depends on $a_n$

$L_p$ : $O(D^3)$ vs. $L_d$ : $O(N^3)$

→ $O(N) - O(N^2)$

# AdaBoost & Ensemble

- Assume we have K classifiers.
- They're independent (errors uncorrelated)
- error $p < 0.5$

Bagging (Bootstrap Aggregation) ∈

- A simple majority vote of all classifiers should have a lower error than each individual classifier.

# Bayesian Model Averaging

$$p(X) = \sum_{h=1}^{H} p(X|h)\, p(h)$$

- Just one model is responsible for generating the entire data set.
- The probability distribution over h just reflects our uncertainty which model that is.
- As the size of the data set increases, this uncertainty reduces, & $p(X|h)$ becomes focused on just one of the models.

| MoG (Model Combination) | Bayesian Model Averaging |
|---|---|
| - Different data points generated by different model components | - Whole data generated by a single model |
| - Uncertainty is about which compon. created which data point. | - Uncertainty is about which model was responsible |
| ⇒ One latent $z_n$ for each point: $p(X) = \prod_{n=1}^{N} p(x_n) = \prod_{n=1}^{N} \sum_{z_n} p(x_n, z_n)$ | ⇒ One latent $z$ for entire data $p(X) = \sum_{z} p(X, z)$ |

## Expected Error

Combine $M$ predictors $y_m(x)$ for target output $h(x)$

$$y_{com}(x) = \frac{1}{M} \sum_{m=1}^{M} y_m(x) \quad : \text{committee}$$

$$y(x) = h(x) + \epsilon(x)$$

$$E_x = \left[ \{ y_m(x) - h(x) \}^2 \right] = E_x[\epsilon_m^2(x)]$$

($E_x$: error)

Average error of individual models : $E_{AV} = \frac{1}{M} \sum_{m=1}^{M} E_x[\epsilon_m(x)^2]$

Average error of committee : $E_{com} = E_x\left[ \left( \frac{1}{M} \sum_{m=1}^{M} y_m(x) - h(x) \right)^2 \right]$

$$= E_x\left[ \left( \frac{1}{M} \sum_{m=1}^{M} \epsilon_m(x) \right)^2 \right]$$

with assumptions:

- $E_x(\epsilon_m(m)) = 0$ zero mean
- $E_x(\epsilon_m(m)\epsilon_j(x)) = 0$ uncorrelated

$\Rightarrow E_{com} = \frac{1}{M} E_{AV}$

↳ In practice : usually highly correlated !

## Adaptive Boosting

- Iteratively select an ensemble of component classifiers
- After each iteration, reweight misclassified training examples.
  - increase the chance of being selected in a sampled training set
  - Increase the misclassification cost when traing on the full set

$h_m(x)$ : weak classifier / base classifier

$H(x)$ : strong classifier / final classifier.

$$H(x) = \text{sign}\left( \sum_{m=1}^{M} \alpha_m h_m(x) \right)$$

# AdaBoost

1. Initialisation : Set $w_n^{(1)} = \frac{1}{N} \quad \forall n = 1 \dots N$

2. For $m = 1 \dots M$ iterations

a) Train a new weak classifier $h_m(x)$ using the current weighting coefficients $W^{(m)}$ by minimising the weighted error function :

$$J_m = \sum_{m=1}^{N} w_n^{(m)} \, I\left(h_m(x) \neq t_n\right)$$

b) Estimate the weighted error of this classifier on $X$ :

$$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} \, I\left(h_m(x) \neq t_n\right)}{\sum_{n=1}^{N} w_n^{(m)}}$$

c) Calculate a weighting coefficient for $h_m(x)$

$$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

d) Update the weighting coefficients :

$$w_n^{(m+1)} = w_n^{(m)} \exp\left\{\alpha_m I\left(h_m(x) \neq t_n\right)\right\}$$

## AdaBoost Summary

- Properties
  - Simple combination of multiple classifiers.
  - Easy to implement.
  - Can be used with many different types of classifiers.
    - None of them needs to be too good on its own.
    - In fact, they only have to be slightly better than chance.
  - Commonly used in many areas.
  - Empirically good generalization capabilities.
- Limitations
  - Original AdaBoost sensitive to misclassified training data points.
    - Because of exponential error function.
    - Improvement by GentleBoost
  - Single-class classifier
    - Multiclass extensions available

# Minimising Exponential Error:

$$E = \sum_{n=1}^{N} \exp\{-t_n f_m(x_n)\}$$

$$= \sum_{n=1}^{N} \exp\left\{\underbrace{-t_n f_{m-1}(x_n)}_{=\text{const.}} - \frac{1}{2} t_n \alpha_m h_m(x_n)\right\}$$

$$= \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(x_n)\right\}$$

$$f_m(x) = \frac{1}{2} \sum_{l=1}^{m} \alpha_l h_l(x)$$

$$f_{m-1}(x) = \frac{1}{2} \sum_{l=1}^{m} \alpha_l h_l(x)$$

$$\Rightarrow f_m(x) = f_{m-1}(x) + \frac{1}{2} \alpha_m h_m(x)$$

**Sequential Minimisation:** Suppose $h_1(x) \dots h_{m-1}(x)$ & $\alpha_1 \dots \alpha_{m-1}$ are fixed $\Rightarrow$ only minimise w.r.t. $\alpha_m$ $h_m(x)$

$$E = e^{-\alpha_m/2} \sum_{n \in T_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in F_m} w_n^{(m)}$$

True: $t_n h_m(x_n) = +1$

False: $t_n h_m(x_n) = -1$

$$= \left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(x_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$$

const. $\qquad \frac{\partial E}{\partial h_m(x_n)} \stackrel{!}{=} 0 \qquad$ const

$\Rightarrow$ equivalent to: $J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(x) \neq t_n)$

$$\frac{\partial E}{\partial \alpha_m} \stackrel{!}{=} 0 \Rightarrow \left(\frac{1}{2} e^{\alpha_m/2} + \frac{1}{2} e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(x_n) \neq t_n) \stackrel{!}{=} \frac{1}{2} e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$$

$$\epsilon_m := \frac{\sum_{n=1}^{N} w_n^{(m)} I(h_m(x) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}} = \frac{e^{-\alpha_m/2}}{e^{\alpha_m/2} + e^{-\alpha_m/2}} = \frac{1}{e^{\alpha_m} + 1}$$

$$\Rightarrow \alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

$$w_n^{(m+1)} = w_n^{(m)} \cdot \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(x_n)\right\} = w_n^{(m)} \cdot \exp\left\{\alpha_m I(h_m(x_n) \neq t_n)\right\}$$

# Perceptron Learning - Learn $\phi$

Linear Output: $y(x) = w^T x + w_0$

Logistic Output: $y(x) = \sigma(w^T x + w_0)$

$\rightsquigarrow$ Generised Multiclass (non-linear):

$$y_k(x) = \sum_{i=0}^{d} w_{ki}\, \phi(x_i) \qquad y_k(x) = \sigma\left( \sum_{i=0}^{d} w_{ki}\, \phi(x_i) \right)$$

$\sigma$: activation; $\phi$: basis

- If the output unit is correct, leave the weights alone.
- If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
- If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.

$$\Rightarrow \quad w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta\,(y_k(x_n; w) - t_{kn})\,\phi_j(x_n)$$

(Delta Rule ! LMS Rule !)

Limitation: - Perceptrons with fixed, hand-coded input features can model any separable function perfectly, given right input features.

- Exponential number of input features

- Once features designed, strong limit on what it can learn

$\Rightarrow$ Learn features !

- L2 loss — $\Rightarrow$ Least-squares regression
  $L(t, y(\mathbf{x})) = \sum_n (y(\mathbf{x}_n) - t_n)^2$
- L1 loss: — $\Rightarrow$ Median regression
  $L(t, y(\mathbf{x})) = \sum_n |y(\mathbf{x}_n) - t_n|$
- Cross-entropy loss — $\Rightarrow$ Logistic regression
  $L(t, y(\mathbf{x})) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$
- Hinge loss — $\Rightarrow$ SVM classification
  $L(t, y(\mathbf{x})) = \sum_n [1 - t_n y(\mathbf{x}_n)]_+$
- Softmax loss — $\Rightarrow$ Multi-class probabilistic classification
  $L(t, y(\mathbf{x})) = -\sum_n \sum_k \left\{ \mathbb{I}(t_n = k) \ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))} \right\}$

# Learning with hidden Units using GD.

$$E(W) = \sum_n L(t_n, y(x_n; W)) + \lambda \Omega(W)$$

$$L(t_n, y(x_n; W)) = \sum_n (y(x_n; W) - t_n)^2 \qquad L_2 \text{ Loss}$$

$$\Omega(W) = \|W\|_F^2 \qquad L_2 \text{ Regn. (weight decay)}$$

Update each weight $W_{ij}^{(k)}$ in the direction of $\frac{\partial E}{\partial w_{ij}^{(k)}}$

## Gradient

1. Naive Analytical Differentiation

   Analytical computation + Chain Rule:
   - with increasing depth, exponential paths! ⇒ Infeasible

2. Numerical Differentiation

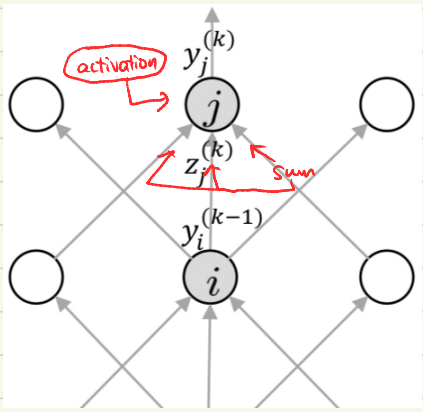
   Inefficient

3. Incremental Analytical Differentiation (Backpropagation)

   ① Convert discrepancy between each output & its target value into an error derivate.

   ② Compute error derivatives in each hidden layer from error derivatives in the layer above.

   ③ Use error derivatives w.r.t. activities to get error derivatives w.r.t. the incoming weights.




$$\frac{\partial E}{\partial z_j^{(k)}} = \frac{\partial E}{\partial y_j^{(k)}} \cdot \frac{\partial y_j^{(k)}}{\partial z_j^{(k)}} = \frac{\partial E}{\partial y_j^{(k)}} \cdot \frac{\partial g(z_j^{(k)})}{\partial z_j^{(k)}}$$

$$\frac{\partial E}{\partial y_i^{(k-1)}} = \sum_j \frac{\partial z_j^{(k)}}{\partial y_i^{(k-1)}} \frac{\partial E}{\partial z_j^{(k)}} = \sum_j w_{ji}^{(k-1)} \frac{\partial E}{\partial z_j^{(k)}}$$

$$\frac{\partial E}{\partial w_{ji}^{(k-1)}} = \frac{\partial z_j^{(k)}}{\partial w_{ji}^{(k-1)}} \cdot \frac{\partial E}{\partial z_j^{(k)}} = y_i^{(k-1)} \frac{\partial E}{\partial z_j^{(k)}}$$

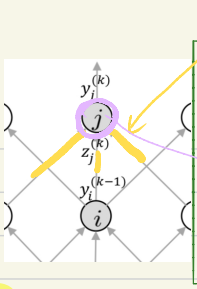
Forward Pass

1. $\frac{\partial E}{\partial y^{(l)}} = \frac{\partial}{\partial y^{(l)}} L(t, y) + \lambda \frac{\partial}{\partial y^{(l)}} \Omega$

2. $\frac{\partial E}{\partial z^{(l)}} = \frac{\partial E}{\partial y^{(l)}} \cdot \frac{\partial y^{(l)}}{\partial z^{(l)}} = \frac{\partial E}{\partial y^{(l)}} \cdot g'(z^{(l)})$

3. $\frac{\partial E}{\partial W^{(l)}} = \frac{\partial E}{\partial z^{(l)}} \cdot y^{(l-1)T} + \lambda \cdot \frac{\partial \Omega}{\partial W^{(l)}}$

4. $\frac{\partial E}{\partial y^{(l-1)}} = W^{(k)T} \cdot \frac{\partial E}{\partial z^{(l)}}$




$z^{(k)} = W^{(k)} y^{(k-1)}$

$y^{(k)} = g_k(z^{(k)})$

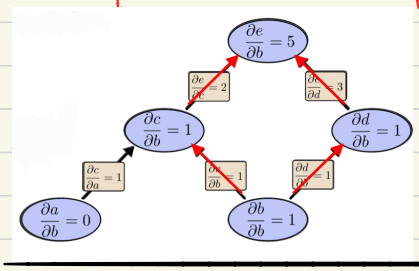
$E = L(t, y) + \lambda \Omega(w$

Forward

Backward

## 4. Automatic Differentiation

### Computational Graph

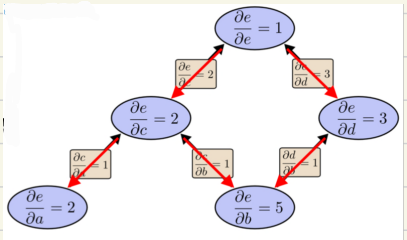



Forward Mode : $O$(# edges)

Derivative of every node w.r.t. b

One Pass / Node.

---




Reverse Mode : $O$(# edges)

Derivative of e w.r.t. every node

Single Pass : Speedup in $O$(# input)

1. $y = \text{module.fprop}(x)$

2. $\frac{\partial E}{\partial x} = \text{module.bprop}\left(\frac{\partial E}{\partial y}\right)$

- Practical issue
  - Exponentials get very big and can have vastly different magnitudes.
  - Trick 1: Do not compute first softmax, then log, but instead directly evaluate log-exp in the nominator and log-sum-exp in the denominator.
  - Trick 2: Softmax has the property that for a fixed vector $\mathbf{b}$
    $$\text{softmax}(\mathbf{a} + \mathbf{b}) = \text{softmax}(\mathbf{a})$$

  $\Rightarrow$ Subtract the largest weight vector $\mathbf{w}_j$ from the others.

$$E(w) = -\sum_{n=1}^{N} \sum_{k=1}^{K} \left\{ \mathbb{I}(t_n = k) \ln \frac{\exp(w_k^T x)}{\sum_{j=1}^{K} \exp(w_j^T x)} \right\}$$

# Gradient Descent

< Compute gradients for each weight
Adjust weights in the direction of gradient

## Batch

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left.\frac{\partial E(w)}{\partial w_{kj}}\right|_{w^{(\tau)}}$$

- Process the full dataset at once to compute gradients

+ Conditions of convergence are well understood.
+ Many acceleration techniques (conjugate gradients) only operate in batch learning
+ Theoretical analysis of weight dynamics & convergence rates are simpler

## Stochastic

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left.\frac{\partial E_n(w)}{\partial w_{kj}}\right|_{w^{(\tau)}}$$

- Choose a single example from the training set
- Compute gradient based on this example
- Noisy, which has some advantages

+ Usually much faster than batch
+ often results in better solutions ?
+ can be used for tracking changes

→ **Minibatch**

* Process only a small batch of training examples together
* Start with a small batch size and increase it as training proceeds

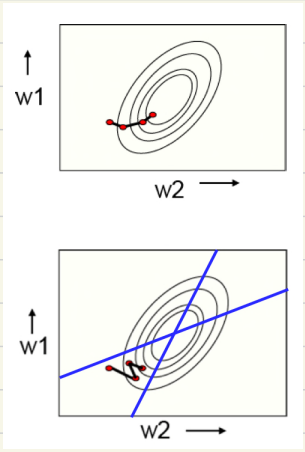
Error function should be normalised by Minibatch size. s.t. keep same learning rate between minibatches

$$E(w) = \frac{1}{N}\sum_n L(t_n, y(x_n; W)) + \frac{1}{N}\Omega(w)$$

+ Gradients will be more stable than SGD still faster than BGD
+ Take advantage of redundancies in the training set
+ Matrix operations are more efficient than vector operations

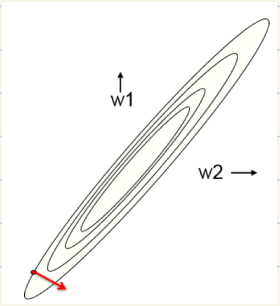
# Learning Rate

$$\eta_{opt} = \left( \frac{d^2 E(W^{(2)})}{dW^2} \right)^{-1}$$




Batch : updates perpendicular to contour lines

Stochastic : updates perpendicular to constraints from training examples.




Inputs are correlated :

The ellipse very elongated :

The direction of steepest descent is almost perpendicular to the dir towards the minimum.

→ Momentum

$$\Delta W = V(t) = \alpha V(t-1) - \varepsilon \frac{\partial E}{\partial W}(t)$$

$$= \alpha \Delta W(t-1) - \varepsilon \frac{\partial E}{\partial W}(t)$$

Techniques : At the beginning of learning :

- use small $\alpha = 0,5$
- Once the large gradients have disappeared raise momentum smoothly to its final values.

Plane surface error : $V(\infty) = \frac{1}{1-\alpha} \left( -\varepsilon \frac{\partial E}{\partial W} \right)$

for $\alpha \to 1$, much faster than simple gradient descent.

Global learning rate, multiplied by a local gain per weight :

Gradients can get very small in the early layers of nets

Fan-in (often varies widely between layers) of a unit determines the size of Overshooting when changing multi. weights simultaneously to correct the same error.

## RMSProp

Motivation:
- The magnitude of gradient can be very different for different weights & can change during learning.
- Hard to choose a single global learning rate
- For batch, use the sign of the gradient ?

Idea: Divide the gradient by a running average of its recent magnitude

$$\text{MeanSq}(w_{ij}, t) = 0.9\,\text{MeanSq}(w_{ij}, t-1) + 0.1\left(\frac{\partial E}{\partial w_{ij}}(t)\right)^2$$

Divide the gradient by $\sqrt{\text{MeanSq}(w_{ij}, t)}$.

AdaGrad / AdaDelta / Adam: less sensitive to parameter setting

Adam: quasi-standard.

## Tricks of the Trade

* Shuffling
* Augmentation: reduce overfitting
  - Cropping
  - Zooming
  - Flipping
  - Colour PCA
* Normalisation

MLP only

- Normalise all inputs that an input unit sees to zero-mean, unit covariance
- if possible, decorrelate them using PCA

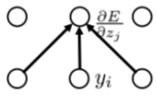
Fast convergence:
- zero-mean
- same covariance
- uncorrelated

- Motivation
  - Consider the Gradient Descent update steps

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left.\frac{\partial E(\mathbf{w})}{\partial w_{kj}}\right|_{\mathbf{w}^{(\tau)}}$$

  - From backpropagation, we know that

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}}\frac{\partial E}{\partial z_j} = y_i \frac{\partial E}{\partial z_j}$$




  - When all of the components of the input vector $y_i$ are positive, all of the updates of weights that feed into a node will be of the same sign.

⇒ Weights can only all increase or decrease together.
⇒ Slow convergence

# Nonlinearities

- Symmetric sigmoids: such as tanh often converge faster than the standard logistic sigmoid: $f = 1.7159 \tanh(\frac{2}{3}x)$

  ⇒ When used with transformed inputs, the variance of the outputs will be close to 1.

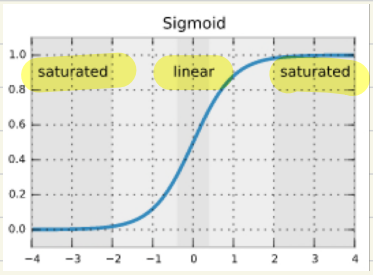
## Output nodes

- Sigmoid for nice probabilistic interpretation (range [0,1])
- tanh for regression tasks

## Internal nodes

- tanh (historically)
  - ↳ better than sigmoid cos symmetry.

→ ReLU

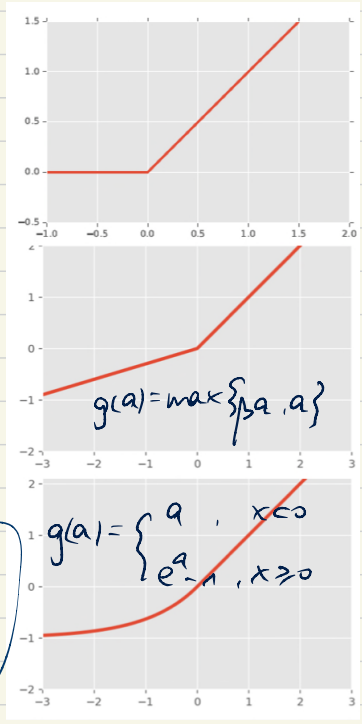



All parameters too small:

- Variance of activations will drop in each layer
- Sigmoids are approx. linear close to 0
- Good for passing gradients through.
  - ↳ But Gradient loss of the nonlinearity.
  - ↳ No benefit of having multiple layers

All parameters become larger:

- They will saturate and gradient → 0




avoid stuck at 0 — weaker offset bias

No offset bias — Need store activations

**ReLU** (de-facto standard)

$g(a) = \max\{0, a\}$, $\frac{\partial g(a)}{\partial a} = \begin{cases} 1, & a > 0 \\ 0, & \text{else} \end{cases}$

+ Much easier to propagate gradients through deep networks
+ No need store ReLU Output separately.

− A certain fraction of units stuck at zero

- if initial weights are chosen s.t. ReLU Output is 0 for the entire training set, the unit will never pass through a gradient to change those weights

**Leaky ReLU**

**ELU**

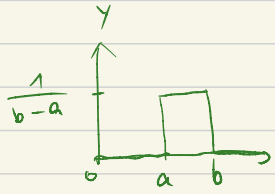
− ReLU has an offset bias, since its outputs will always be positive!

# Initialisation of Weights

- Assuming that < the training set has been normalised
  $f(x) = 1.7159 \tanh(\frac{2}{3}x)$ is used

- The initial weights should be randomly drawn from distribution (e.g. uniform or normal) with mean zero & variance $\sigma_w^2 = \frac{1}{n_{IN}}$

  $n_{IN}$: fan-in (# connections into the node)




pdf: $f(x) = \begin{cases} \frac{1}{b-a} & , [a,b] \\ 0 & , \text{else} \end{cases}$

cdf: $F(x) = \begin{cases} 0 & , <a \\ 1 & , >b \\ \frac{x-a}{b-a} & , \text{else} \end{cases}$

$E(X) = \int x f(x)\, dx$

$$E(X) = \int_a^b x \cdot \frac{1}{b-a} dx = \frac{1}{b-a} \cdot \frac{1}{2} x^2 \Big|_a^b = \frac{1}{2}(b-a)$$

$$E(X^2) = \int_a^b x^2 \frac{1}{b-a} dx = \frac{1}{b-a} \frac{1}{3} x^3 \Big|_a^b = \frac{1}{3}(b-a)^2$$

$$Var(X) = \frac{1}{3}(b-a)^2 - \left(\frac{1}{2}(b-a)\right)^2 = \left(\frac{1}{3} - \frac{1}{4}\right)(b-a)^2 = \frac{1}{12}(b-a)^2$$

$$SD(X) = \frac{1}{\sqrt{12}}(b-a)$$

$$\frac{1}{12}(b-a)^2 = \frac{1}{n_{IN}} \Rightarrow W \sim U\left[-\frac{\sqrt{3}}{\sqrt{n_{IN}}}, \frac{\sqrt{3}}{\sqrt{n_{IN}}}\right]$$

or w.r.t. Fan-in & Fan-out: $W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_{IN}+n_{OUT}}}, \frac{\sqrt{6}}{\sqrt{n_{IN}+n_{OUT}}}\right]$

↑ Based on tanh units: linearity assumption around zero.

He et al.: for ReLU: $Var(W) = \frac{2}{n_{IN}}$

# Batch Normalisation

Motivation: Optim. works best if all inputs of a layer are normed.

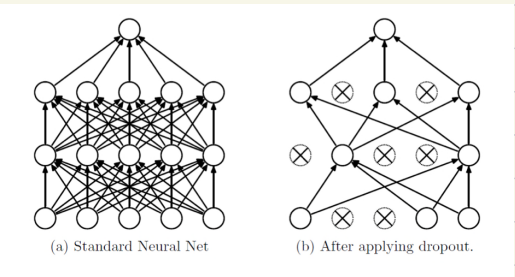
Idea: perform transformations on all activations & undo them when backproping gradients.

Complication: centering + normalisation also needs to be done at test time, but minibatch no longer available

- Learning normalisation parameters to compensate for the expected bias of the previous layer. (moving average)

Effect:
- Much improved convergence (but para important)
- widely used

# Dropout



(a) Standard Neural Net (b) After applying dropout.

Randomly switch off units during training (sort of Regularisation)

- Change network architecture of each minibatch effectively training many different variants of the network.
- When applying the trained network, multiply activations with the probability that the unit was set to zero during training.

⇒ Greatly improved performance.

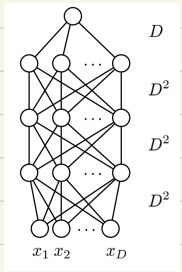
# CNN

- Hierarchical Multi-Layer ?
  - Visual scenes are hierarchically organized.
  - Biological vision is hierarchical too.
  - Shallow architectures are inefficient at representing complex functions

## FCN

#Para

$|\theta| = 3D^2 + D$




for 32x32 Image:

$D = 32^2$

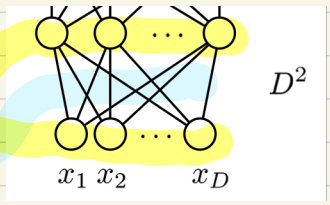
$\Rightarrow |\theta| = 3 \cdot 32^4 + 32^2 \approx 3 \cdot 10^6$

↳ Hard to train, Need to initialise carefully.

For 1000 x 1000 Image:

1M Hidden units per layer

1T Para per layer



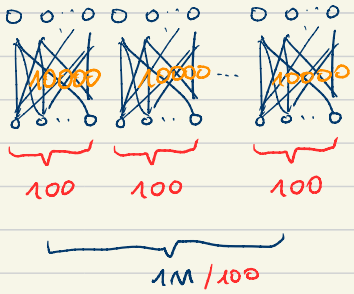

## Local FCN

10x10 Receptive fields

⇓

100M Para

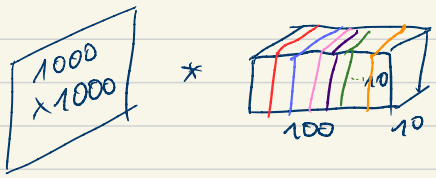
$= \frac{1M}{100} \cdot 100^2$




## CNN

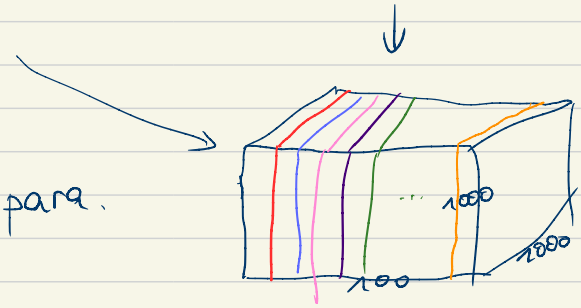
100 Filters 10x10

100 x 10x10 = 10K Para




Response map:

1000 x1000 x100




Only memory, not para.

# Depth, Parameters, Stride, Max Pooling ...

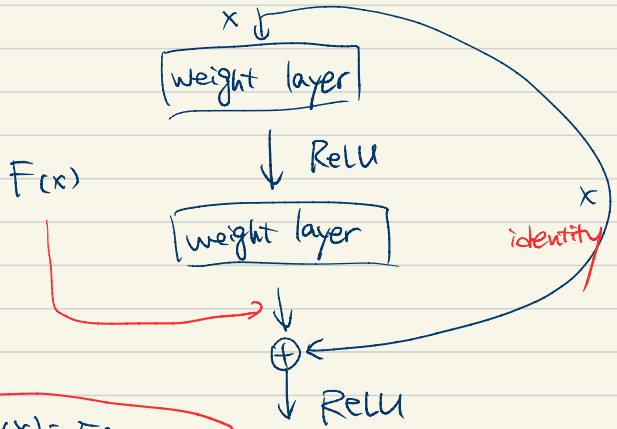
## Architecture

LeNet AlexNet VGGNet GoogleNet Residual

AlexNet: 11x11, stride 4 — 3x3 stride 1

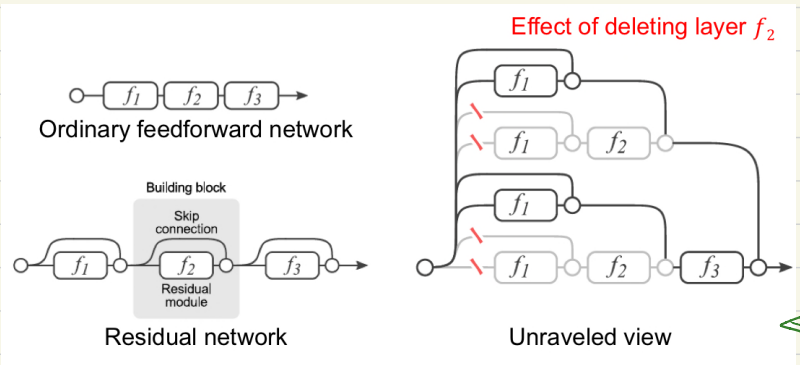
- Stack 3x3 on top of another 3x3 ⇒ 5x5 receptive field
- 3x3 three ⇒ 7x7
- But much fewer parameters $3 \cdot 3^2 = 27$, $7^2 = 49$
- In addition: non-linearity in-between 3x3 layers for additional discriminativity.

## Res Net




$H(x) = F(x) + x$

+ if identity optimal: easy to set weights as 0
+ if optimal mapping closer to identity, easy to find small fluctuations
+ direct path for the gradient to flow to the previous stages




## Summary ResNet:

+ The effective path in ResNets are relatively shallow. (5-17)
+ Resilience to deletion:

Deleting any single layer only affects a subset of paths, & the shorter ones less than the longer

New interpretation:
- ResNets work by creating an ensemble of relatively shallow paths
- Deeper → larger ensemble
- excluding longer paths doesn't negatively affect results

# Word Embedding

$h = W^T \cdot x$

- $h$: embeddings, $dx1$, ~(50, 300)
- $W^T$: LUT, $Vxd$
- $x$: one-hot vec, $Vx1$, ~1M

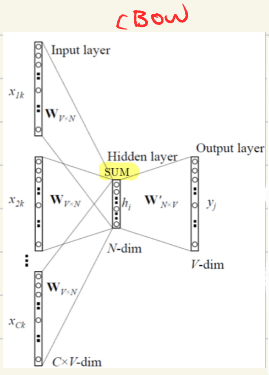
↝ Full Connect.

↳ Huge Para.

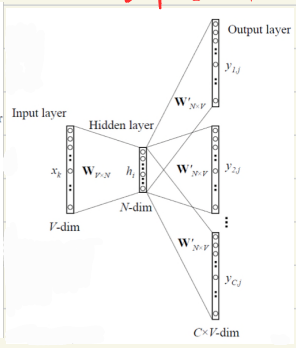
word2vec < CBOW, Skip-gram → fewer parameters

CBOW < predict current work.

Skip-gram < predict words within a certain range



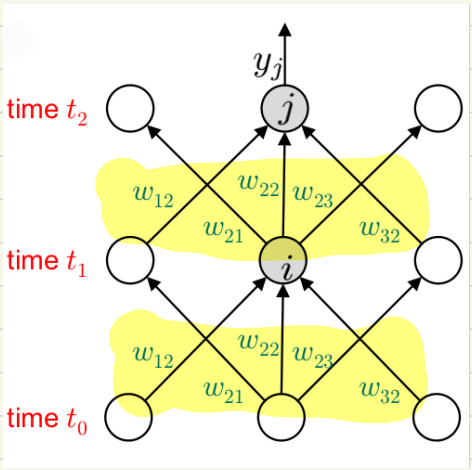

Skip Gram




→ Embedding preserves linear regularity

↳ Hierarchical Softmax

# RNN

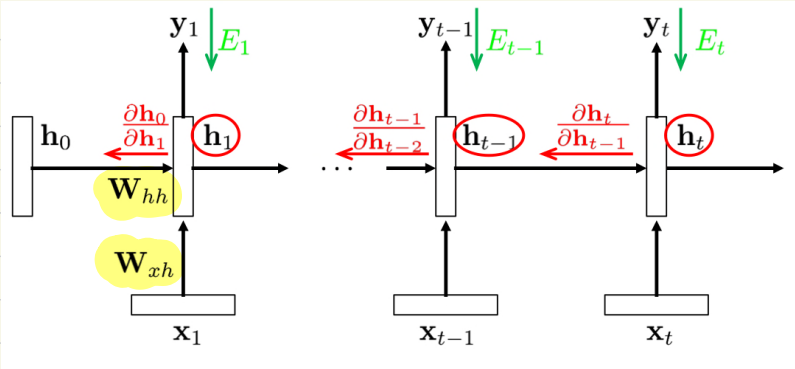



RNN : just a feedforward net that keeps reusing the same weights

Backprop : $w_1 = w_2 \leftarrow \nabla w_1 = \nabla w_2$

$\frac{\partial E}{\partial w_1} + \frac{\partial E}{\partial w_2}$ for both $w_1$ & $w_2$.

# BPTT Backpropagation Through Time




Inputs : $x_t$

Outputs : $y_t$

Hidden Units : $h_t$

Initial State : $h_0$

Connection : $W_{xh}$, $W_{hy}$, $W_{hh}$

$$\begin{cases} h_t = \sigma(W_{xh} x_t + W_{hh} h_{t-1} + b) \\ \hat{y}_t = \text{softmax}(W_{hy} h_t) \end{cases}$$

$E = \sum_t E_t$ : error sum over time.

For some weight: $\frac{\partial E_t}{\partial w_{ij}} = \frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial w_{ij}} + \frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial h_{t-1}}\frac{\partial h_{t-1}}{\partial w_{ij}} + \cdots$ 偏微分

$$= \sum_{1 \le k \le t} \left( \frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

immediate p'd : $h_{k-1}$ const.

$$= \prod_{t \ge i \ge k} \frac{\partial h_i}{\partial h_{i-1}} = \prod_{t \ge i \ge k} W_{hh}^T \, \text{diag}(\sigma'(h_{i-1}))$$

$= (W_{hh}^T)^l$, for $t \to \infty$, $l = t-k$.

Exploding/Vanishing Gradient:

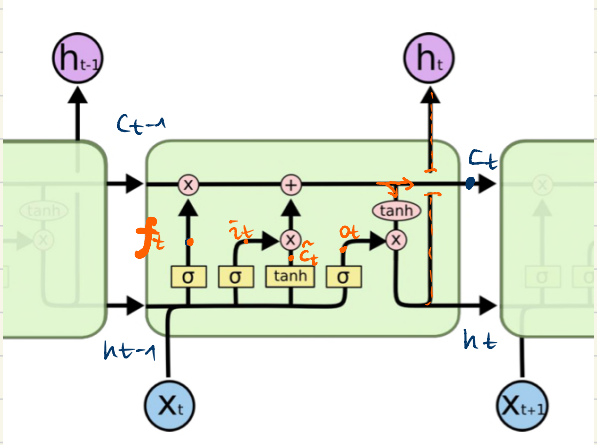
For $W_{hh}$: Largest eigenvalue $< 1$ vanishing, $> 1$ exploding

Gradient Clipping: if $\|\hat{g}\| \ge$ threshold : $\hat{g} \leftarrow \frac{\text{threshold}}{\|\hat{g}\|} \cdot \hat{g}$

- Glorot / He
- ReLU
- LSTM, GRU

BPTT : Dependency between long distance :

↳ LSTM




C : Cell State
h : hidden Units

σ : sigmoid [0,1]

tanh : [-1,1]

$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$ | forget

$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$

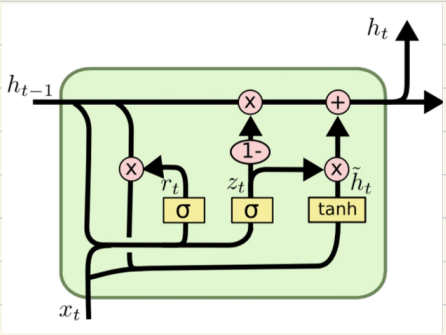
$\tilde{C}_t = \tanh(W_c \cdot [h_{t-1}, x_t] + b_c)$ | update

$C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t$

$o_t = \sigma(W_o [h_{t-1}, x_t] + b_o)$ | output

$h_t = \tanh(C_t) \cdot o_t$

Gated Recurrent Units




$z_t = \sigma(W_z \cdot [h_{t-1}, x_t])$ update

$r_t = \sigma(W_r \cdot [h_{t-1}, x_t])$ reset

$\tilde{h}_t = \tanh(W \cdot [r_t * h_{t-1}, x_t])$

$h_t = h_{t-1} \cdot (1 - z_t) + z_t \cdot \tilde{h}_t$

# Repetition

## 1. Bayes Decision Theory

- Prior, Likelihood, Posterior = $\frac{\text{Likelihood} \times \text{Prior}}{\text{Normalised Factor}}$

| | | |
|---|---|---|
| $p(a)$ | $p(x\|a)$ | $p(a\|x)$ |
| $p(b)$ | $p(x\|b)$ | $p(b\|x)$ |
| Result | Given results Predict feature Architecture data | Given feature architecture data Predict results / labels |

- Optimal decision Rule → Likelihood-Ratio-Test

Decide for $C_1$, if $p(C_1|x) > p(C_2|x)$

$$\Leftrightarrow p(x|C_1)\,p(C_1) > p(x|C_2)\,p(C_2) \Leftrightarrow \frac{p(x|C_1)}{p(x|C_2)} > \underbrace{\frac{p(C_2)}{p(C_1)}}_{\theta}$$

- Minimising Expected Loss

$$E(L) = \sum_k \sum_j \int_{R_j} L_{kj}\, p(x, C_k)\, dx$$

Choosing Regions $R_j$ such that $E(L) = \sum_k L_{kj}\, p(C_k|x)$

$E(L)$: Expected Loss; $L_{kj}$: Loss; $p(C_k|x)$: Posterior

## 2. Probability Desity Estimation

Gaussian: $$N(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$N(x|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2}\,|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right\}$$

- Maximum Likelihood Approach.

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

Log-Likelihood

$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

$$\frac{\partial}{\partial \theta} E(\theta) = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \theta} p(x_n|\theta)}{p(x_n|\theta)} \stackrel{!}{=} 0$$

Non-parametric Solutions : Histogram : $p_i = \frac{n_i}{N \Delta_i}$

Kernel Density Estimation : $p(x) \simeq \frac{K}{NV}$

fixed V determine K → Kernel (window, Gaussian...)

fixed K, determine V → KNN

3. Mixture Models (MoG)

$$p(j) = \pi_j \cdot p(x|\theta_j) \quad , \quad p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j) \underbrace{p(j)}_{\text{weights}}$$

→ Iterative Strategy. ( Prior knowledge missing)

K-Means Clustering : - Local, - results initialisation dependent

1. Initialisation : pick K arbitrary centroids : cluster means
2. Assign each sample to the closest centroid.
3. Adjust the centroids to be the means of the samples assigned to them
4. Go to 2 until no change.

↳ EM ( Expectation - Maximisation) - Local

(E) Softly assign samples to mixture components.

$$\gamma_j(x_n) \leftarrow \frac{\pi_j \, N(x_n|\mu_j, \Sigma_j)}{\sum_{k=1}^{N} \pi_k \, N(x_n|\mu_k, \Sigma_k)} \qquad \forall j = 1..K, \; n = 1..N$$

(M) : Re-estimate the parameters ( separately for each mixture components) based on the soft assignments

$$\hat{N}_j \leftarrow \sum_{n=1}^{N} \gamma_j(x_n) \quad = \text{soft number of samples labled } j$$

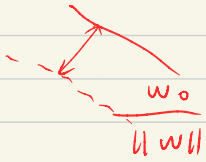
$$\hat{\pi}_j^{new} \leftarrow \frac{\hat{N}_j}{N}$$

$$\hat{\mu}_j^{new} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(x_n)\, x_n$$

$$\hat{\Sigma}_j^{new} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(x_n)\,(x_n - \hat{\mu}_j^{new})(x_n - \hat{\mu}_j^{new})^T$$

## 4. Linear Discriminant Functions ( Decision ! )

$$y(x) = w^T x + w_0$$




### Least - Squares ( sum-of-Squares Error : Closed form ! )

$$E(w) = \sum_{n=1}^{N} (y(x_n; w) - t_n)^2$$

$$\rightsquigarrow E_D(\tilde{w}) = \frac{1}{2} Tr\{(\tilde{X}\tilde{w} - T)^T (\tilde{X}\tilde{w} - T)\} \Rightarrow \tilde{W} = (\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T T = \tilde{X}^{\dagger} T$$

$$\Rightarrow y(x) = \tilde{w}^T \tilde{x} = T^T (\tilde{X}^{\dagger})^T \tilde{x}$$

↳ sensitive to outliers

↳ Generalized Linear Models. $y(x) = g(w^T x + w_0)$

↓ activation function (nonlinear)

If $g$ is monotonous, the resulting decision boundaries are still linear function of $x$

↳ With non-linear Basis functions

$$y(x) = \sum_{j=1}^{M} w_j \phi_j(x) + w_{k0}$$

\+ Nonlinear decision boundaries

\+ choosing right $\phi_j$, every continuous func. can be approxi.

\- No closed form → GD

## Probabilistic Discriminative Models (logistic regression)

+ Probabilistic interpretation but discriminative method: only focus on decision hp
+ Advantageous for High-dim

$$p(t|w) = \prod_{n=1}^{N} y_n^{t_n} \{1-y_n\}^{1-t_n} \quad \text{with} \quad y_n = p(C_1|\phi_n)$$

$$E(w) = -\ln p(t|w) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$

cross-entropy error

$$= -\sum_{n=1}^{N}\sum_{k=0}^{1} \{\mathbb{I}(t_n = k) \ln P(y_n = k|x_n; w)\}$$

multi class → Softmax : $\frac{\exp(a_k)}{\sum_i \exp(a_i)}$

$$E(w) = -\sum_{n=1}^{N}\sum_{k=1}^{K} \left\{\mathbb{I}(t_n = k) \ln \frac{\exp(w_k^T x)}{\sum_{j=1}^{K} \exp(w_j^T x)}\right\}$$

$$\nabla_{w_k} E(w) = -\sum_{n=1}^{N} [\mathbb{I}(t_n = k) \ln P(y_n = k|x_n; w)]$$

## 5. SVM

Primal : $L_p = \frac{1}{2}\|w\|^2 - \sum_{n=1}^{N} a_n \{t_n y(x_n) - 1\}$

KKT : $a_n \geq 0$

$t_n y(x_n) - 1 \geq 0$

$a_n \{t_n y(x_n) - 1\} = 0$

$\lambda \geq 0$
$f(x) \geq 0$
$\lambda f(x) = 0$

$\forall a_n > 0 : t_n y(x_n) - 1 \geq 0 \Rightarrow$ Supporting Vectors

☆ Dual : $L_D(a) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (x_m^T x_n)$

$a_n \geq 0 \quad \forall n$

$\sum_{n=1}^{N} a_n t_n = 0$

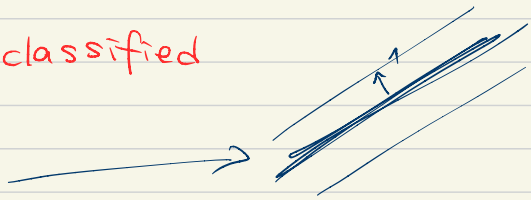
Comparison: $L_d$ only depends on $a_n$

$L_p$ : $O(D^3)$ vs. $L_d$ : $O(N^3)$

$\rightarrow O(N) - O(N^2)$

Slack Variable for Non-Separable

$$\xi_n = \begin{cases} 0, & \text{correct} \\ |t_n - y(x_n)|, & \text{misclassified} \end{cases}$$



Points on desicion boundary: $\xi_n = 1$

$$\Rightarrow L_d(a) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m (x_n^T x_m)$$

$$\begin{cases} 0 \le a_n \le C \\ \sum_{n=1}^{N} a_n t_n = 0 \end{cases}$$

Kernel Trick: $y(x) = w^T \phi(x) + b = \sum_{n=1}^{N} a_n t_n \phi(x_n)^T \phi(x) + b$

$$k(x, y) = \phi(x)^T \phi(y)$$

$$L_d(a) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(x_m, x_n)$$

$$\begin{cases} 0 \le a_n \le C \\ \sum_{n=1}^{N} a_n t_n = 0 \end{cases}$$