Linear methods of classification

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Linear discriminant functions

- Classification of two classes ω_1 and ω_2.
- Linear discriminant function:

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

- Decision rule:

$$x \rightarrow \begin{cases} \omega_1, & g(x) \geq 0 \\ \omega_2, & g(x) < 0 \end{cases}$$

- Decision boundary $B = \{x : g(x) = 0\}$

Properties

- $x_A, x_B \in B \Rightarrow \begin{cases} g(x_A) = w^T x_A + w_0 = 0 \\ g(x_B) = w^T x_B + w_0 = 0 \end{cases} \Rightarrow$ $w^T(x_A - x_B) = 0$, so $w \perp B$.
- Distance from the origin to B is equal to absolute value of the projection of $x \in B$ on $\frac{w}{\|w\|}$:

$$\langle x, \frac{w}{\|w\|} \rangle = \frac{\langle x, w \rangle}{\|w\|} = \{w^T x + w_0 = 0\} = -\frac{w_0}{\|w\|}$$

- So $\rho(0, B) = \frac{w_0}{\|w\|}$, and w_0 determines the offset from the origin.

Distance from x to B

Denote $x_\perp$ - the projection of x on B, and $r = \langle \frac{w}{\|w\|}, x - x_\perp \rangle$ - the signed length of the orthogonal complement of x on B:

$$x = x_\perp + r\frac{w}{\|w\|}$$

After multiplication by w and addition of w_0:

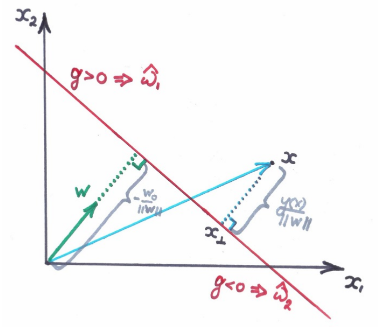
$$w^T x + w_0 = w^T x_\perp + w_0 + r\frac{\langle w, w\rangle}{\|w\|}$$

Using $w^T x + w_0 = g(x)$ and $w^T x_\perp + w_0 = 0$, we obtain:

$$r = \frac{g(x)}{\|w\|}$$

So from one side of the hyperplane $r > 0 \Leftrightarrow g(x) > 0$, and from the other side of the hyperplane $r < 0 \Leftrightarrow g(x) < 0$.

Illustration



Linear decision rule:

$$\widehat{c}(x) = \begin{cases} \omega_1, & g(x) > 0 \\ \omega_2, & g(x) < 0 \end{cases}$$

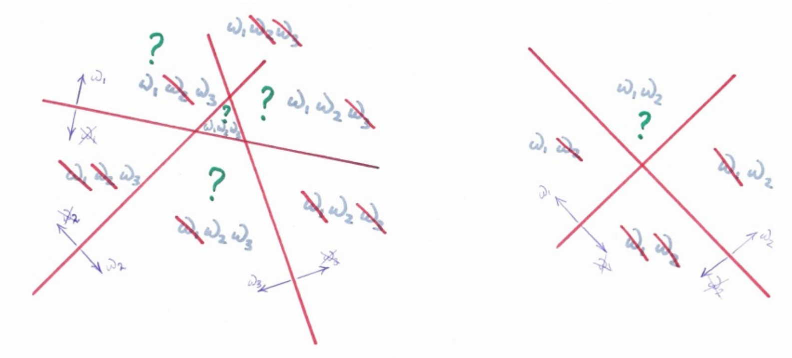
Decision boundary: $g(x) = 0$, confidence of decision: $|g(x)| / \|w\|$.

Multiple classification

- Popular schemes:
    - one versus all
    - one versus rest
- If only sign is taken into account, they have regions of ambiguity.

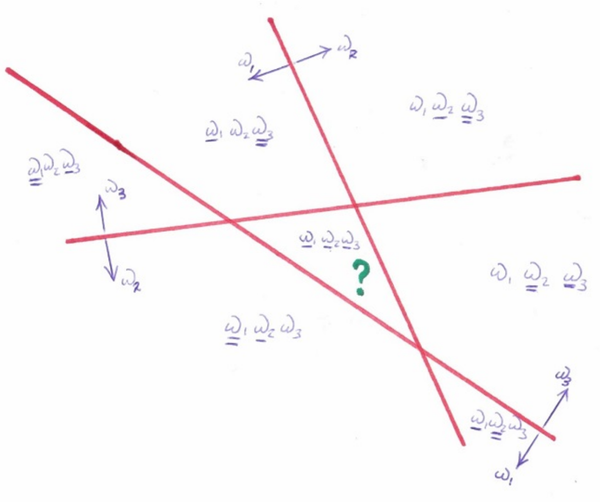
One versus all - ambiguity

Classification among three classes: $\omega_1, \omega_2, \omega_3$



One versus one - ambiguity

Classification among three classes: $\omega_1, \omega_2, \omega_3$



Multiple classes classification - solution

- Classification among $\omega_1, \omega_2, ...\omega_C$.
- Use C discriminant functions $g_c(x) = w_c^T x + w_{c0}$
- Decision rule:

$$\widehat{c}(x) = \arg\max_c g_c(x)$$

- Decision boundary between classes ω_i and ω_j is linear:

$$\left(w_i - w_j\right)^T x + \left(w_{i0} - w_{j0}\right) = 0$$

- Decision regions are convex.

Proof of convexity of decision regions

Suppose $\widehat{c}(x_A) = \widehat{c}(x_B) = c$, which by definition means, that

$$\begin{aligned} w_c^T x_A + w_{c0} &\geq w_k^T x + w_{k0} \quad \forall k \neq c \qquad (1) \\ w_c^T x_B + w_{c0} &\geq w_k^T x + w_{k0} \quad \forall k \neq c \qquad (2) \end{aligned}$$

For $\lambda x_A + (1-\lambda)x_B$, $\lambda \in (0,1)$ by summing (1) and (2) with weights λ and $(1-\lambda)$, we obtain:

$$w_c^T\left(\lambda x_A + (1-\lambda)x_B\right) + w_{c0} \geq w_k^T\left(\lambda x_A + (1-\lambda)x_B\right) + w_{k0} \quad \forall k \neq c$$

which means that $\widehat{c}\left(\lambda x_A + (1-\lambda)x_B\right) = c$ and decision region for every $c = 1, 2, \ldots C$ is convex.

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Linear discriminant functions

- Consider binary classification of classes ω_1 and ω_2.
- Denote classes ω_1 and ω_2 with $y = +1$ and $y = -1$.
- Linear discriminant function: $g(x) = w^T x + w_0$,

$$\widehat{\omega} = \begin{cases} \omega_1, & g(x) \geq 0 \\ \omega_2, & g(x) < 0 \end{cases}$$

- Decision rule: $y = \operatorname{sign} g(x)$.
- Define constant feature $x_0 \equiv 1$, then $g(x) = w^T x = \langle w, x \rangle$ for $w = [w_0, w_1, ..w_D]^T$.
- Define the margin $M(x) = g(x)y$
  - $M(x) \geq 0$ <=> object x is correctly classified
  - $|M(x)|$ - confidence of decision

Weights selection

- Target: minimization of the number of misclassifications:

$$Q_{accurate}(w|X) = \sum_i \mathbb{I}[M(x_i|w) < 0] \to \min_w$$

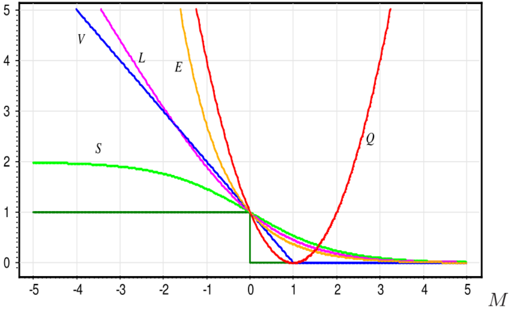
- Problem: standard optimization methods are inapplicable, because $Q(w, X)$ is discontinuous.
- Idea: approximate loss function with smooth function $\mathcal{L}$:

$$\mathbb{I}[M(x_i|w) < 0] \le \mathcal{L}(M(x_i|w))$$

Approximation of the target criteria

We obtain the upper boundary on the empirical risk:

$$\begin{aligned} Q_{accurate}(w|X) &= \sum_i \mathbb{I}[M(x_i|w) < 0] \\ &\le \sum_i \mathcal{L}(M(x_i|w)) = Q_{approx}(w|X) \end{aligned}$$



$$Q(M) = (1-M)^2$$
$$V(M) = (1-M)_+$$
$$S(M) = 2(1+e^M)^{-1}$$
$$L(M) = \log_2(1+e^{-M})$$
$$E(M) = e^{-M}$$

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Optimization

- Optimization task to obtain the weights:

$$
\begin{aligned}
F(w) &= Q_{approx}(w|X,Y) = \sum_{i=1}^{n} \mathcal{L}(M(x_i, y_i|w)) \\
&= \sum_{i=1}^{n} \mathcal{L}(\langle w, x_i \rangle y_i) \to \min_{w}
\end{aligned}
$$

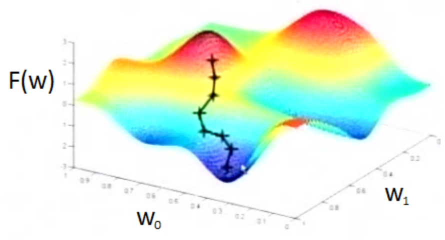
- Gradient descend algorithm:

INPUT:
η - parameter, controlling the speed of convergence
stopping rule

ALGORITHM:
initialize w_0 randomly
while stopping rule is not satisfied:
    $w_{n+1} \leftarrow w_n - \eta \frac{\partial F(w_n)}{\partial w}$
    $n \leftarrow n+1$

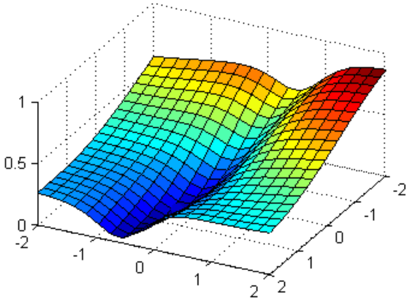
Gradient descend

- Possible stopping rules:
  - $|w_{n+1} - w_n| < \varepsilon$
  - $|F(w_{n+1}) - F(w_n)| < \varepsilon$
  - $n > n_{max}$
- Suboptimal method of minimization in the direction of the greatest reduction of $F(w)$:



Recommendations for use

- Convergence is faster for normalized features
  - feature normalization solves the problem of «elongated valleys»



Convergence acceleration

Stochastic gradient descend method

set the initial approximation w_0
calculate $\widehat{Q}_{approx} = \sum_{i=1}^{n} \mathcal{L}(M(x_i|w_0))$
iteratively until convergence $\widehat{Q}_{approx}$:

1. select random pair (x_i, y_i)
2. recalculate weights: $w_{n+1} \leftarrow w_n - \eta_n \mathcal{L}'(\langle w_n, x_i \rangle y_i) x_i y_i$
3. estimate the error: $\varepsilon_i = \mathcal{L}(\langle w_{n+1}, x_i \rangle y_i)$
4. recalculate the loss $\widehat{Q}_{approx} = (1-\alpha)\widehat{Q}_{approx} + \alpha\varepsilon_i$
5. $n \leftarrow n + 1$

Variants for selecting initial weights

- $w_0 = w_1 = ... = w_D = 0$
- For logistic $\mathcal{L}$ (because the horizontal asymptotes):
  - randomly on the interval $[-\frac{1}{2D}, \frac{1}{2D}]$
- For other functions $\mathcal{L}$:
  - randomly
- $w_i = \frac{\langle x^i, y\rangle}{\langle x^i, x^i\rangle}$

Discussion of SGD

Advantages

- Easy to implement
- Works online
- A small subset of learning objects may be sufficient for accurate estimation

Discussion of SGD

Advantages

- Easy to implement
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Drawbacks

- Suboptimal - converges to local optimum
- Needs selection of η_n:
  - too big: divergence
  - too small: very slow convergence
- Overfitting possible for large D and small N
- When $\mathcal{L}(u)$ has left horizontal asymptotes (e.g. logistic), the algorithm may «get stuck» for large values of $\langle w, x_i \rangle$.

Examples

Delta rule $\mathcal{L}(M) = (M-1)^2$

$$w \leftarrow w - \eta(\langle w, x_i \rangle - y_i)x_i$$

The same rule applies for linear regression $f(x) = \langle w, x \rangle$ with the loss function $(\langle w, x \rangle - y)^2$, $y \in \mathbb{R}$

$\mathcal{L}(M) = [-M]_+$

Perceptron of Rosenblatt

$$w \leftarrow w + \begin{cases} 0, & \langle w, x_i \rangle y_i \geq 0 \\ \eta x_i y_i & \langle w, x_i \rangle y_i < 0 \end{cases}$$

Natural rule but it does not try to widen the gap between classes.

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Regularization for SGD

- L_2-regularization for upperbound approximation:

$$Q_{approx}^{regularized}(w) = Q_{approx}(w) + \frac{\tau}{2}|w|^2$$

- SGD weights modification: $w \leftarrow w(1-\eta\tau) - \eta Q'_{approx}(w)$

Regularization

- Useful technique to control the trade-off between bias and variance, can be applied to any algorithm.

$$Q^{regularized}(w) = Q(w) + \tau ||w||_2$$

$$Q^{regularized}(w) = Q(w) + \tau ||w||_1$$

$$||w||_1 = \sum_{d=1}^{D} |w^d|, \quad ||w||_2 = \sqrt{\sum_{d=1}^{D} (w^d)^2}$$

- Examples:
  - LASSO: least-squares regression, using $||w||_1$
  - Ridge: least-squares regression, using $||w||_2$
  - Elastic Net: : least-squares regression, using both

L_1 norm

- $||w||_1$ regularizer will do feature selection.
- Consider
$$Q(w)=\sum_{i=1}^{n}\mathcal{L}_i(w)+\frac{1}{C}\sum_{d=1}^{D}|w_d|$$
- if $\frac{1}{C}>\sup_w\left|\frac{\partial\mathcal{L}(w)}{\partial w_i}\right|$, then it becomes optimal to set $w_i=0$
- For smaller C more inequalities will become active.

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Maximum probability estimation

- $X=\{x_1,x_2,...x_n\}$, $Y=\{y_1,y_2,...y_n\}$ - training sample of i.i.d. observations, $(x_i,y_i)\sim p(y|x,w)$
- ML estimation $\widehat{w}=\arg\max_w p(Y|X,w)$
- Using independence assumption:

$$\prod_{i=1}^{n}p(y_i|x_i,w)=\sum_{i=1}^{n}\ln p(y_i|x_i,w)\to\max_w$$

- Approximated misclassification:

$$\sum_{i=1}^{n}\mathcal{L}(g(x_i)y_i|w)\to\min_w$$

- Interrelation:

$$\mathcal{L}(g(x_i)y_i|w)=-\ln p(y_i|x_i,w)$$

Maximum a prosteriori estimation

- $X=\{x_1,x_2,...x_n\}$, $Y=\{y_1,y_2,...y_n\}$ - training sample of i.i.d. observations, $(x_i,y_i)\sim p(x,y|w)$
- $x_i\sim p(x|w)$
- MAP estimation:
  - w is random with prior probability $p(w)$

$$p(w|X,Y)=\frac{p(X,Y,w)}{p(X,Y)}=\frac{p(X,Y|w)p(w)}{p(X,Y)}\propto p(X,Y|w)p(w)$$

$$w=\arg\max_w p(w|X,Y)=\arg\max_w p(X,Y|w)p(w)$$

$$\sum_{i=1}^{n}\ln p(x_i,y_i|\theta)+\ln p(w)\to\max_w$$

Gaussian prior

- Gaussian prior

$$\ln p(w,\sigma^2)=\ln\left(\frac{1}{(2\pi\sigma^2)^{n/2}}e^{-\frac{||w||_2^2}{2\sigma^2}}\right)=-\frac{1}{2\sigma^2}||w||_2^2+\text{const}(w)$$

- Laplace prior

$$\ln p(w,C)=\ln\left(\frac{1}{(2C)^n}e^{-\frac{||w||_1}{C}}\right)=-\frac{1}{C}||w||_1+\text{const}(w)$$

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Logistic regression

Add constant to x, add w_0 to w. $\sigma(z)=\frac{1}{1+e^{-z}}$
Two-class classification:

$$score(\omega_1|x)=w^T x$$

$$p(\omega_1|x)=\sigma(w^T x)$$

Multiple class classification:

$$\begin{cases} score(\omega_1|x)=w_1^T x \\ score(\omega_2|x)=w_2^T x \\ \cdots \\ score(\omega_C|x)=w_C^T x \end{cases}$$

Logistic regression

Probabilities are obtained using soft-max:

$$p(\omega_c|x) = \frac{exp(w_c^T x)}{\sum_i exp(w_i^T x)}$$

w_c, $c = 1, 2, ...C$ defined up to shift v:

$$\frac{exp((w_c - v)^T x)}{\sum_i exp((w_i - v)^T x)} = \frac{exp(-v^T x)exp(w_c^T x)}{\sum_i exp(-v^T x)exp(w_i^T x)}$$

Take $v = w_C$, obtain previous formula.

Logistic regression

Assume (γ_1, γ_2 are the costs of misclassifying classes ω_1 and ω_2):

$$\ln\left(\frac{\gamma_1 p(\omega_1|x)}{\gamma_2 p(\omega_2|x)}\right) = \beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}$$

It is equivalent to

$$\begin{aligned} p(\omega_2|x) &= \frac{1}{1 + exp(\beta_0' + \boldsymbol{\beta}^T \boldsymbol{x})} \\ p(\omega_1|x) &= \frac{exp(\beta_0' + \boldsymbol{\beta}^T \boldsymbol{x})}{1 + exp(\beta_0' + \boldsymbol{\beta}^T \boldsymbol{x})} \end{aligned}$$

where $\beta_0' = \beta_0 - \ln(\gamma_1/\gamma_2)$

Logistic regression

Decision rule (following Bayes minimum risk principle):

$$x = \begin{cases} \omega_1, & \beta_0' + \boldsymbol{\beta}^T \boldsymbol{x} > 0 \\ \omega_2, & \beta_0' + \boldsymbol{\beta}^T \boldsymbol{x} < 0 \end{cases}$$

Estimate with ML:

$$\prod_{i=1}^{n} p(c_i | x_i) \to \max_{\beta_0', \boldsymbol{\beta}}$$

where c_i is the class of x_i.

Multiclass logistic regression

- Assumption:

$$\ln\left(\frac{\gamma_s p(\omega_s|x)}{\gamma_C p(\omega_C|x)}\right) = \beta_{s0} + \beta_s^T \boldsymbol{x}, \quad s = 1, 2, ...C-1$$

- Posterior class probabilities:

$$\begin{aligned} p(\omega_s|x) &= \frac{exp(\beta'_{s0} + \beta_s^T x)}{1 + \sum_{s=1}^{C-1} exp(\beta'_{s0} + \beta_s^T x)}, \quad s = 1, 2, ...C-1 \\ p(\omega_C|x) &= \frac{1}{1 + \sum_{s=1}^{C-1} exp(\beta'_{s0} + \beta_s^T x)} \end{aligned}$$

$$\beta'_{s0} = \beta_{s0} - \ln(\gamma_s/\gamma_C)$$

Multiclass logistic regression

- Decision rule (following Bayes minimum risk principle): assign x to class $c = \arg\max_c \beta_{c0} + \beta_c^T x$ if $\beta_{c0} + \beta_c^T x > 0$ otherwise assign x to class C.
- Estimate with ML:

$$\prod_{i=1}^{n} p(c_i|x_i) \to \max_{\beta_0', \boldsymbol{\beta}}$$

  where c_i is the class of x_i.
- Please pay attention to the difference between β_0 and β_0'.

Loss function for logistic regression

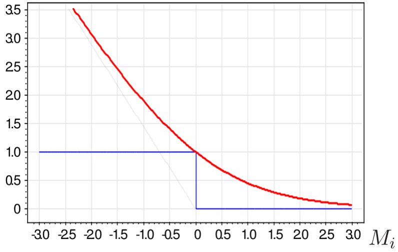
For two class situation $p(y|x) = \sigma(\langle w, x\rangle y)$ for $\sigma = \frac{1}{1+e^{-z}}$, $w = [\beta_0', \beta]$, $x = [1, x_1, x_2, ...x_D]$.

Estimation with ML:

$$\prod_{i=1}^{n} \sigma(\langle w, x_i\rangle y_i) \to \max_w$$

which is equivalent to

$$\sum_i^n \ln(1 + e^{-\langle w, x_i\rangle y_i}) \to \min_w$$



It follows that logistic regression is linear discriminant estimated with loss function $\mathcal{L}(M) = \ln(1 + e^{-M})$.

SGD realization of logistic regression

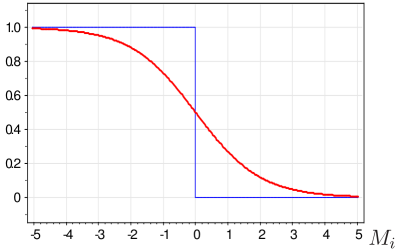
Substituting $\mathcal{L}(M) = \ln(1 + e^{-M})$ into update rule, we obtain that for each sample (x_i, y_i) weights should be adapted according to

$$w \leftarrow w + \eta\sigma(-M_i)x_i y_i$$

Perceptron of Rosenblatt update rule:

$$w \leftarrow w + \eta\mathbb{I}[M_i < 0]x_i y_i$$

- Logistic rule update is the smoothed variant of perceptron's update.
- The more severe the error (according to margin) - the more weights are adapted.



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Problem statement

- Standard linear classification decision rule

$$\widehat{c} = \begin{cases} 1, & w^T x \geq -w_0 \\ 2, & w^T x < w_0 \end{cases}$$

  is equivalent to

  1. dimensionality reduction to 1-dimensinal space (defined by w)
  2. making classification in this space

- Idea of Fisher's LDA: find direction, giving most discriminative projections.

Possible realization

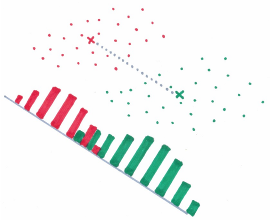
- Classification between ω_1 and ω_2.
- Define $C_1 = \{i : x_i \in \omega_1\}, \quad C_2 = \{i : x_i \in \omega_2\}$ and

$$m_1 = \frac{1}{N_1}\sum_{n\in C_1} x_n, \quad m_2 = \frac{1}{N_1}\sum_{n\in C_2} x_n$$

$$\mu_1 = w^T m_1, \quad \mu_2 = w^T m_2$$

Naive solution:

$$\begin{cases}(\mu_1 - \mu_2)^2 \to \max_w \\ \|w\| = 1\end{cases}$$

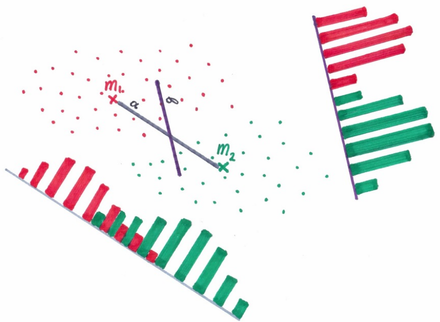


Fisher's LDA

- Define projected within class variances:

$$s_1 = \sum_{n \in C_1} (w^T x_n - w^T m_1)^2, \quad s_2 = \sum_{n \in C_2} (w^T x_n - w^T m_2)^2$$

- Fisher's LDA criterion: $\frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2} \to \max_w$



Equivalent representation

$$\frac{(\mu_1-\mu_2)^2}{s_1^2+s_2^2}=\frac{\left(w^T m_1-w^T m_2\right)^2}{\sum_{n\in C_1}(w^T x_n-w^T m_1)^2+\sum_{n\in C_2}(w^T x_n-w^T m_2)^2}$$

$$=\frac{\left[w^T(m_1-m_2)\right]^2}{\sum_{n\in C_1}\left[w^T(x_n-m_1)\right]^2+\sum_{n\in C_2}\left[w^T(x_n-m_1)\right]^2}$$

$$=\frac{w^T(m_1-m_2)(m_1-m_2)^T w}{w^T\left[\sum_{n\in C_1}(x_n-m_1)(x_n-m_1)^T+\sum_{n\in C_2}(x_n-m_2)(x_n-m_2)^T\right]w}$$

$$=\frac{w^T S_B w}{w^T S_W w}$$

$$\begin{aligned} S_B &= (m_1-m_2)(m_1-m_2)^T, \\ S_W &= \sum_{n\in C_1}(x_n-m_1)(x_n-m_1)^T+\sum_{n\in C_2}(x_n-m_2)(x_n-m_2)^T \end{aligned}$$

Fisher's LDA solution

$Q(w) = \frac{w^T S_B w}{w^T S_W w} \to \max_w$
Using property that $\frac{d}{dw}\left(w^T A w\right) = 2Aw$ for any $A \in \mathbb{R}^{KxK}$, $A^T = A$

$$\frac{dQ(w)}{dw} \propto 2S_B w \left[w^T S_W w\right] - 2\left[w^T S_B w\right] S_W w = 0$$

which is equivalent to

$$\left[w^T S_W w\right] S_B w = \left[w^T S_B w\right] S_W w$$

So

$$w \propto S_W^{-1} S_B w \propto S_W^{-1}(m_1 - m_2)$$