Linear methods of classification

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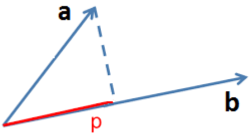
Reminder

1. $a = [a^1, ...a^D]^T$, $b = [b^1, ...b^D]^T$
2. Scalar product $\langle a, b \rangle = a^T b = \sum_{d=1}^{D} a_d b_b$
3. $a \perp b$ means that $\langle a, b \rangle = 0$
4. Norm $\|a\| = \sqrt{\langle a, a \rangle}$
5. Distance $\rho(a, b) = \|a - b\| = \sqrt{\langle a - b, a - b \rangle}$



- $p = \langle a, \frac{b}{\|b\|} \rangle$
- $|p| = \left| a, \frac{b}{\|b\|} \right|$- unsigned projection length

Orthogonal vector to hyperplane

Theorem 1

Vector w is orthogonal to hyperplane $w^T x + w_0 = 0$

Proof. Consider arbitrary $x_A, x_B \in \{x : \; w^T x + w_0 = 0\}$:

$$w^T x_A + w_0 = 0 \tag{1}$$
$$w^T x_B + w_0 = 0 \tag{2}$$

By substracting (2) from (1), obtain $w^T (x_A - x_B) = 0$, so w is orthogonal to hyperplane. □

Distance from point to hyperplane

Theorem 2

Distance from point x to hyperplane $w^T x + w_0 = 0$ is equal to $\frac{w^T x + w_0}{\|w_0\|}$.

Proof. Project x on the hyperplane, let the projection be p and complement $h = x - p$, orthogonal to hyperplane. Then

$$x = p + h$$

Since p lies on the hyperplane,

$$w^T p + w_0 = 0$$

Since h is orthogonal to hyperplane and according to theorem 1

$$h = r\frac{w}{\|w\|},\ r \in \mathbb{R} \text{ - distance to hyperplane.}$$

Distance from point to hyperplane

$$x = p + r\frac{w}{\|w\|}$$

After multiplication by w and addition of w_0:

$$w^T x + w_0 = w^T p + w_0 + r\frac{w^T w}{\|w\|} = r\|w\|$$

because $w^T p + w_0 = 0$ and $\|w\| = \sqrt{w^T w}$. So we get, that

$$r = \frac{w^T x + w_0}{\|w\|}$$

Comments:

- From one side of hyperplane $r > 0 \Leftrightarrow w^T x + w_0 > 0$
- From the other side $r < 0 \Leftrightarrow w^T x + w_0 < 0$.
- Distance from hyperplane to origin 0 is $\frac{w_0}{\|w\|}$. So w_0 accounts for hyperplane offset.

Binary linear classifier geometric interpretation

Binary linear classifier:

$$\widehat{y}(x) = \text{sign}\left(w^T x + w_0\right)$$

divides feature space by hyperplane $w^T x + w_0 = 0$.

- Confidence of decision is proportional to distance to hyperplane $\frac{|w^T x + w_0|}{\|w\|}$.
- $w^T x + w_0$ is the confidence that class is positive.

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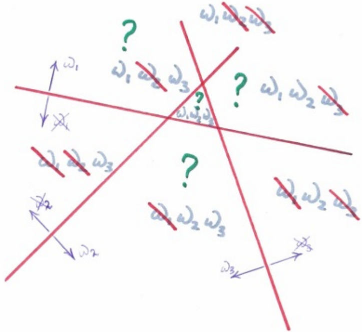
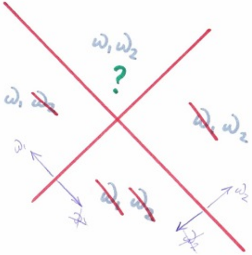
Multiclass classification with binary classifiers

- Task - make C-class classification using many binary classifiers.
- Approaches:
  - **one-versus-all**
    - for each $c = 1, 2, ...C$ train binary classifier on all objects and output $\mathbb{I}[y_n = c]$,
    - assign class, getting the highest score in resulting C classifiers.
  - **one-versus-one**
    - for each $i, j \in [1, 2, ...C]$, $i \neq j$ learn on objects with $y_n \in \{i, j\}$ with output y_n
    - assign class, getting the highest score in resulting $C(C-1)/2$ classifiers.
  - **error correcting codes**

One versus all - ambiguity

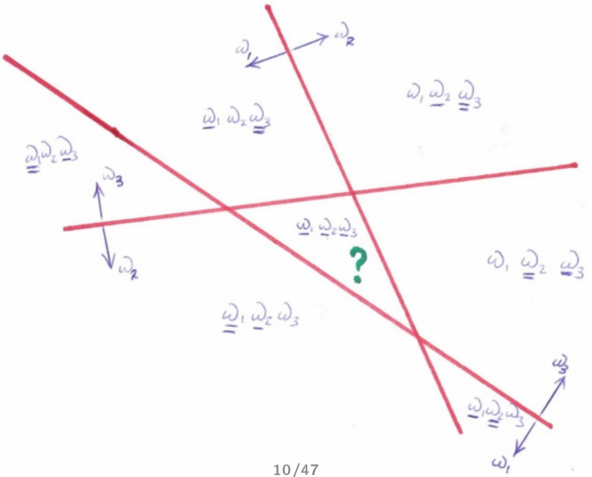
Classification among three classes: $\omega_1, \omega_2, \omega_3$





One versus one - ambiguity

Classification among three classes $\omega_1, \omega_2, \omega_3$ depending only on halfspace may be ambiguous:



Error correcting codes

- Used in classification
- Each class ω_i is coded as a binary codeword W_i consisting of B bits:

$$\omega_i \to W_i$$

- Minimum sufficient amount of bits to code C classes is $\lceil \log_2 C \rceil$
- Given x, B binary classifiers predict each bit of the class codeword.
- Class is predicted as

$$\hat{c}(x) = \arg\min_c \sum_{b=1}^{B} |W_{cb} - \widehat{p}_b(x)|$$

- where W_{cb} is the b-th bit of codeword, corresponding to class c.
- More bits are used to make classification more robust to errors of individual binary classifiers.
- Codewords are selected to have maximum mutual Hamming distance or randomly.

Linear classifier

- Classification among classes 1,2,...C.
- Use C discriminant functions $g_c(x) = w_c^T x + w_{c0}$
- Decision rule:

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

- Decision boundary between classes $y = i$ and $y = j$ is linear:

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

- Decision regions are convex[1].

[1] why? prove that.

Binary linear classifier

- For two classes $y \in \{+1, -1\}$ classifier becomes

$$\widehat{y}(x) = \begin{cases} +1, & w_{+1}^T x + w_{+1,0} > w_{-1}^T x + w_{-1,0} \\ -1 & \text{otherwise} \end{cases}$$

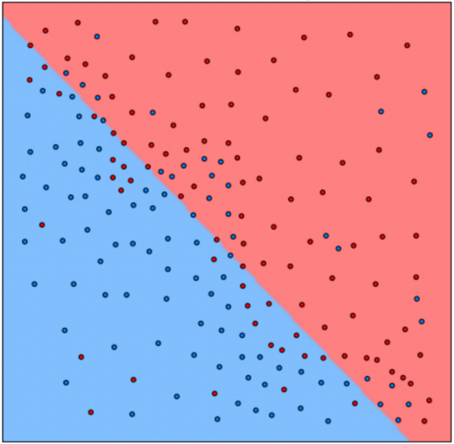
- This decision rule is equivalent to

$$\begin{aligned} \widehat{y}(x) &= \text{sign}(w_{+1}^T x + w_{+1,0} - w_{-1}^T x + w_{-1,0}) = \\ &= \text{sign}\left(\left(w_{+1}^T - w_{-1}^T\right) x + (w_{+1,0} - w_{-1,0})\right) \\ &= \text{sign}\left(w^T x + w_0\right) \end{aligned}$$

for $w = w_{+1} - w_{-1}$, $w_0 = w_{+1,0} - w_{-1,0}$.

- Decision boundary $w^T x + w_0 = 0$ is linear.
- Multiclass case can be solved using multiple binary classifiers with one-vs-all, one-vs-one or error correcting codes schemes.

Example: linear decision region



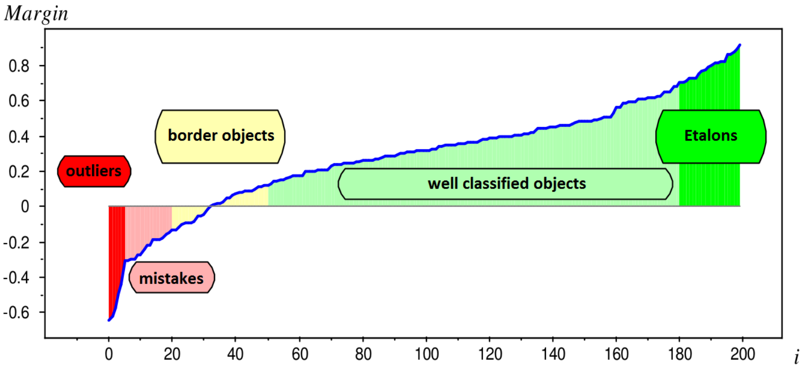
Margin of binary linear classifier

$$\begin{aligned} M(x,y) &= g_y(x) - g_{-y}(x) = w_y^T x + w_{y,0} - w_{-y}^T x - w_{-y,0} \\ &= [w_y - w_{-y}]^T x + [w_{y,0} - w_{-y,0}] \\ &= y\left([w_{+1} - w_{-1}]^T x + [w_{+1,0} - w_{-1,0}]\right) \\ &= y\left(w^T x + w_0\right) \end{aligned}$$

- Margin=score, how well classifier predicted true y for object x.
- $M(x,y|w) > 0$ <=> object x is correctly classified as y
    - signs of $w^T x + w_0$ and y coincide
- $|M(x,y|w)| = \left|w^T x + w_0\right|$ - confidence of decision
    - proportional to distance from x to hyperplane $w^T x + w_0 = 0$.

Margin

Objects, ordered by margin



Redefinitions

- Add w_0 to $w = [w_1, ...w_D]^T$:

$$w = [w_0, w_1, ...w_D]^T$$

- Add constant feature $x_0 \equiv 1$ to $x = [x^1, ...x^D]^T$:

$$x = [1, x^1, ...x^D]^T$$

- Binary linear classifier becomes:

$$\widehat{y}(x) = \text{sign}\left(w^T x\right)$$

- Margin becomes:

$$M(x, y|w) = w^T xy$$

Weights optimization

- Margin=score, how well classifier predicted true y for object x.
- Task: select such w to increase $M(x_n, y_n|w)$ for all n.
- Formalization:

$$\frac{1}{N}\sum_{n=1}^{N}\mathcal{L}\left(M(x_n, y_n|w)\right) \to \min_{w}$$

Misclassification rate optimization

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$$\frac{1}{N}\sum_{n=1}^{N}\mathbb{I}[M(x_n, y_n|w) < 0] \to \min_{w}$$

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is not recommended:

  - discontinious function, can't use numerical optimization!
  - continous margin is more informative than binary error indicator.

Misclassification rate optimization

- Misclassification rate optimization:

$$\frac{1}{N}\sum_{n=1}^{N}\mathbb{I}[M(x_n, y_n|w) < 0] \to \min_w$$

is not recommended:

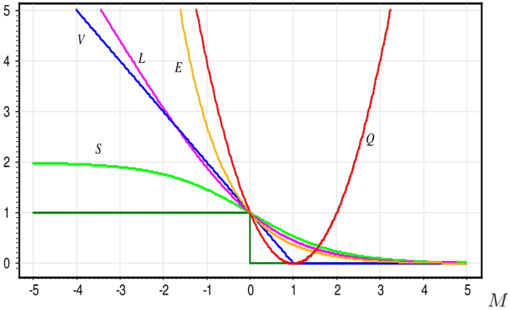
  - discontinious function, can't use numerical optimization!
  - continous margin is more informative than binary error indicator.

- If we select loss function $\mathcal{L}(M)$ such that $\mathbb{I}[M] \le \mathcal{L}(M)$ then we can optimize upper bound on misclassification rate:

$$\text{MISCLASSIFICATION RATE} = \frac{1}{N}\sum_{n=1}^{N}\mathbb{I}[M(x_n, y_n|w) < 0]$$

$$\le \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}(M(x_n, y_n|w)) = L(w)$$

Common loss functions



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

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Gradient

- For any function $f(x)$, depending from $x = (x_1, ...x_D)^T$ gradient

$$\nabla f(x) := \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \cdots \\ \frac{\partial f(x)}{\partial x_D} \end{pmatrix}$$

- If function $f(x, y)$ depends on other variables y gradient ∇_x considers only derivatives with respect to x:

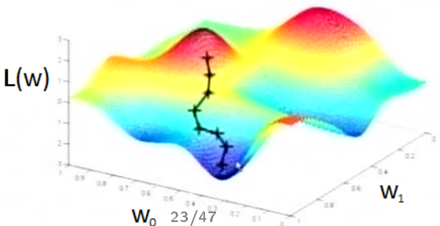
$$\nabla_x f(x, y) := \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \cdots \\ \frac{\partial f(x)}{\partial x_D} \end{pmatrix}$$

Gradient descend optimization

- Optimization task to obtain the weights:

$$L(w) \;=\; \sum_{i=1}^{N} \mathcal{L}(w^T x_i y_i) \to \min_w$$

- For convex $\mathcal{L}(u)$ $L(w)$ will also be convex => method will converge to global optimum from any starting conditions.
- Gradient descend - iterative movement in direction of $-\nabla_w F(w)$.
- Example for $w = (w_0, w_1)^T$:



Gradient descend optimization

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

ALGORITHM:
initialize w_0 randomly
WHILE stopping rule is not satisfied:
    w_{n+1} ← w_n − η∇_w L(w_n)
    n ← n + 1

RETURN w_n
```

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

ALGORITHM:
initialize w_0 randomly
WHILE stopping rule is not satisfied:
$w_{n+1} \leftarrow w_n - \eta \nabla_w L(w_n)$
$n \leftarrow n+1$

RETURN w_n

Any computational issues for big data?

Gradient descend optimization

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

ALGORITHM:
initialize w_0 randomly
WHILE stopping rule is not satisfied:
    w_{n+1} ← w_n − η (1/N) Σ_{i=1}^{N} ∇_w L(x_i, y_i | w_n)
    n ← n + 1

RETURN w_n
```

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

ALGORITHM:
initialize w_0 randomly
WHILE stopping rule is not satisfied:

$$w_{n+1} \leftarrow w_n - \eta \frac{1}{N} \sum_{i=1}^{N} \nabla_w \mathcal{L}(x_i, y_i | w_n)$$

$$n \leftarrow n + 1$$

RETURN w_n

Gradient calculation requires $O(N)$ operations!

Stochastic gradient descent optimization

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

ALGORITHM:
initialize w_0 randomly
WHILE stopping rule is not satisfied:
  randomly sample $I = \{i_1, ...i_K\}$ from $\{1, 2, ...N\}$
  $w_{n+1} \leftarrow w_n - \eta \frac{1}{K} \sum_{i \in I} \nabla_w \mathcal{L}(x_i, y_i | w_n)$
  $n \leftarrow n + 1$

RETURN w_n

Stochastic gradient descent optimization

- Main idea: for random subsample $I = \{i_1, ... i_K\}$, called minibatch,

$$\frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(x_i, y_i|w) \approx \frac{1}{K}\sum_{i\in I}\mathcal{L}(x_i, y_i|w), \quad K \ll N$$

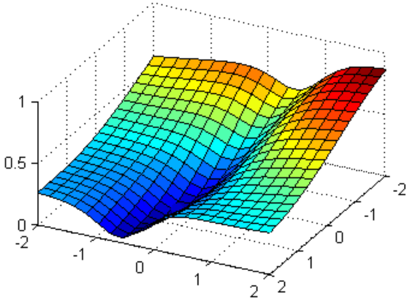
- Original method used $K = 1$.
- $K > 1$ gives smoother gradient. $\frac{1}{K}\sum_{i\in I}\nabla_w\mathcal{L}(x_i, y_i|w_n)$ can still be computed in $O(1)$ because processors internally perform vector arithmetics.
- SGD converges almost surely when $\eta_n \to 0$ as $n \to \infty$ at an appropriate rate.
- In practice η=small const or $\eta_n = \frac{1}{n}$
- Indices generation: before each pass through the training set, it is randomly shuffled and then passed sequentially.

Gradient descend optimization

- Possible stopping rules:
  - $|w_{n+1} - w_n| < \varepsilon$
  - $|L(w_{n+1}) - L(w_n)| < \varepsilon$
  - $n > n_{max}$
- For regression GD and SGD are also applicable: $\mathcal{L}(M(x_n, y_n|w))$ replace with $\mathcal{L}(w^T x_n - y_n)$.

Recommendations for use

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

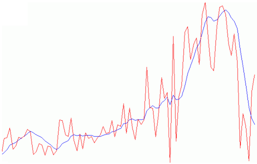


Tracking convergence of SGD

- Estimation of $L(w_n) = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(x_i, y_i|w_n)$ on each iteration takes $O(N)$ and is impractical.
- For series $z_1, ...z_N$ exponentially smoothed series is obtained by

$$\begin{cases} s_1 = z_1 & \alpha \in (0,1) \text{ - hyperparameter} \\ s_{n+1} = \alpha z_{n+1} + (1-\alpha)s_n & \text{recalculation takes } O(1) \end{cases}$$

Example: original (red) and exp-smoother (blue) time series:



Tracking convergence of SGD

Exponential smoothing of loss enables loss reestimation in $O(1)$:

$$L_0^{smooth} = \sum_{i=1}^{N} \mathcal{L}(M(x_i, y_i | w_0))$$
$$L_{n+1}^{smooth} = \alpha \mathcal{L}(M(x_i, y_i | w_0)) + (1-\alpha) L_n^{smooth}$$

Discussion of SGD

Advantages

- Simple
- Works online
- A small subset of learning objects may be sufficient for accurate estimation

Discussion of SGD

Advantages

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Drawbacks

- Optimization using 2nd order derivatives converges faster.
- Needs selection of η_n:
  - too big: divergence
  - too small: very slow convergence
- When $\mathcal{L}(u)$ has horizontal asymptotes (e.g. sigmoid), may «get stuck» for large values of $w^T x_i$.

- If $\mathcal{L}(\cdot)$ is convex => convergence to global min from any starting point.
- If $\mathcal{L}(\cdot)$ is non-convex => convergence to different local min, depending on starting point.

Examples

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

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

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

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

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Regularization

- Insert additional requirement for regularizer $R(\beta)$ to be small:

$$\sum_{n=1}^{N} \mathcal{L}\left(M(x_n, y_n|w) + \lambda R(\beta) \to \min_{\beta}\right.$$

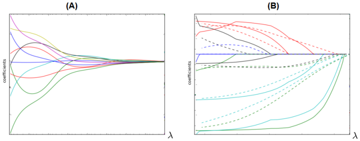
- $\lambda > 0$ - hyperparameter.
- $R(\beta)$ penalizes complexity of models.

$$\begin{array}{ll} R(\beta) = ||\beta||_1 & L_1 \text{ regularization} \\ R(\beta) = ||\beta||_2^2 & L_2 \text{ regularization} \end{array}$$

- Not only *accuracy* matters for the solution but also *model simplicity*!
- λ controls complexity of the model: $\uparrow \lambda \Leftrightarrow$ complexity$\downarrow$.

Comments

- Dependency of β from λ for L_2 (A) and L_1 (B) regularization:



- L_1 can be used for automatic feature selection.
- λ is usually found using cross-validation on exponential grid, e.g. $[10^{-6}, 10^{-5}, ...10^5, 10^6]$.
- It's always recommended to use regularization because
  - it gives smooth control over model complexity.
  - reduces ambiguity for multiple solutions case.

ElasticNet

- ElasticNet:

$$R(\beta) = \alpha||\beta||_1 + (1-\alpha)||\beta||_2^2 \to \min_\beta$$

$\alpha \in (0,1)$ - hyperparameter, controlling impact of each part.

- If two features $x^i$and x^j are equal:
  - L_1 may take only one of them
  - L_2 will take both with equal weight
    - but it doesn't remove useless features
  - ElasticNet both removes useless features but gives equal weight for usefull equal features
    - good, because feature equality may be due to chance on this particular training set

Different account for different features

- Traditional approach regularizes all features uniformly:

$$\sum_{n=1}^{N}\mathcal{L}\left(M(x_n, y_n|w)\right)+\lambda R(\beta)\to\min_{w}$$

- Suppose we have K groups of features with indices:

$$I_1, I_2, ... I_K$$

- We may control the impact of each feature group by minimizing:

$$\sum_{n=1}^{N}\mathcal{L}\left(M(x_n, y_n|w)\right)+\lambda_1 R(\{\beta_i|i\in I_1\})+...+\lambda_K R(\{\beta_i|i\in I_K\})$$

- $\lambda_1, \lambda_2, ... \lambda_K$ can be set using cross-validation
- In practice use common regularizer but with different feature scaling.

L_1 regularization

- $||w||_1$ regularizer will do feature selection.
- Consider

$$L(w)=\sum_{n=1}^{N}\mathcal{L}\left(M(x_n,y_n|w)\right)+\lambda\sum_{d=1}^{D}|w_d|$$

$$\frac{\partial}{\partial w_i}L(w)=\sum_{n=1}^{N}\frac{\partial}{\partial w_i}\mathcal{L}\left(M(x_n,y_n|w)\right)+\lambda\,\mathrm{sign}\,w_i$$

$$\lambda\,\mathrm{sign}\,w_i\nrightarrow 0\text{ when }w_i\to 0$$

- If $\lambda>\max_w\left|\sum_{n=1}^{N}\frac{\partial}{\partial w_i}\mathcal{L}\left(M(x_n,y_n|w)\right)\right|$, then it becomes optimal to set $w_i=0$
- For higher λ more weights become zero.

L_2 regularization

$$L(w) = \sum_{n=1}^{N} \mathcal{L}\left(M(x_n, y_n|w)\right) + \lambda \sum_{d=1}^{D} w_d^2$$

$$\frac{\partial}{\partial w_i} L(w) = \sum_{n=1}^{N} \frac{\partial}{\partial w_i} \mathcal{L}\left(M(x_n, y_n|w)\right) + 2\lambda w_i$$

$$2\lambda w_i \to 0 \text{ when } w_d \to 0$$

- Strength of regularization $\to 0$ as weights $\to 0$.
- So L_2 regularization will not set weights exactly to 0.

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Binary classification

- Linear classifier:

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

- +relationship between score and class probability is assumed:

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

where $\sigma(z) = \frac{1}{1+e^{-z}}$ - sigmoid function

Binary classification: estimation

Using the property $1 - \sigma(z) = \sigma(-z)$ obtain that

$$p(y = +1|x) = \sigma(w^T x) \Longrightarrow p(y = -1|x) = \sigma(-w^T x)$$

So for $y \in \{+1, -1\}$

$$p(y|x) = \sigma(y\langle w, x\rangle)$$

Therefore ML estimation can be written as:

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

Loss function for 2-class logistic regression

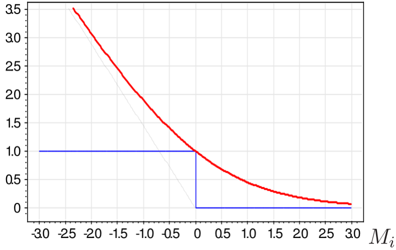
For binary classification $p(y|x) = \sigma(\langle w, x\rangle y)$ $w = [\beta_0', \beta]$, $x = [1, x_1, x_2, ...x_D]$.

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 $\mathcal{L}(M) = \ln(1 + e^{-M})$.

Multiple classes

Multiple class classification:

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

+relationship between score and class probability is assumed:

$$p(\omega_c|x) = softmax(w_c^T x | x_1^T x, ... x_C^T x) = \frac{exp(w_c^T x)}{\sum_i exp(w_i^T x)}$$

Multiple classes

Weights ambiguity:

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

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

To remove ambiguity usually $v = w_C$ is subtracted.

Estimation with ML:

$$\begin{cases} \prod_{n=1}^N softmax(w_{y_n}^T x_n | x_1^T x, ... x_C^T x) \to \max_{w_1, ... w_{C-1}} \\ w_C = \mathbf{0} \end{cases}$$

Summary

- Linear classifier - classifier with linear discriminant functions.
- Binary linear classifier: $\widehat{y}(x) = \text{sign}(w^T x + w_0)$.
- Perceptron, logistic, SVM - linear classifiers estimated with different loss functions.
- Weights are selected to minimize total loss on margins.
- Gradient descent iteratively optimizes $L(w)$ in the direction of maximum descent.
- Stochastic gradient descent approximates $\nabla_w L$ by averaging gradients over small subset of objects.
- Regularization gives smooth control over model complexity.
- L_1 regularization automatically selects features.