Lecture 2: Supervised Learning — Classification

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Intro. to Stats. Machine Learning
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- What's machine learning?
- Randomness is not your enemy.
- All you care is the testing error (not the training error).
- Train too well is not good (overfitting).
- The simplest model that fits the data is also the most plausible (Occam's Razor).

Main types of SL

We have (input, correct output) in the training data, *i.e.* Input-output data pairs $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$.

Based on the output y_i (not the input), SL can be categorised into 3 main types:

- Classification (discrete output)
- Novelty detection (discrete output)
- Regression (continuous output)

Classification

Discrete output y

1. Binary classification $y \in \{-1, 1\}$
2. Multi-class $y \in \{1, 2, \cdots, c\}$ for c classes
3. Multi-label $y = (y^{(1)}, \cdots, y^{(i)}, \cdots y^{(L)})$, where $y^{(i)} \in \{1, 2, \cdots, c_i\}$ assuming L labels and c_i classes for the i-th label.
4. Structured output. Complex objects with examples to show later.

Predict Annual Income (Binary classification)

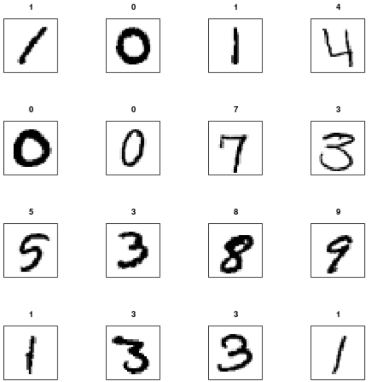
Predict whether income exceeds $50K/yr based on census data.
$y \in \{-1, 1\}$. 1 means $> 50K/yr$, -1 means $\leq 50K/yr$.

Input x from the UCI Adult Dataset

age: continuous.
workclass: Private, Self-emp-not-inc, Self-emp-inc, Federal-gov, Local-gov, State-gov, Without-pay, Never-worked.
fnlwgt: continuous.
education: Bachelors, Some-college, 11th, HS-grad, Prof-school, Assoc-acdm, Assoc-voc, 9th, 7th-8th, 12th, Masters, 1st-4th, 10th, Doctorate, 5th-6th, Preschool.
education-num: continuous.
marital-status: Married-civ-spouse, Divorced, Never-married, Separated, Widowed, Married-spouse-absent, Married-AF-spouse.
occupation: Tech-support, Craft-repair, Other-service, Sales, Exec-managerial, Prof-specialty, Handlers-cleaners, Machine-op-inspct, Adm-clerical, Farming-fishing, Transport-moving, Priv-house-serv, Protective-serv, Armed-Forces.
relationship: Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried.
race: White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black.
sex: Female, Male.
capital-gain: continuous.
capital-loss: continuous.
hours-per-week: continuous.

Handwritten Digits Recognition (Multi-class)

$y \in \{0, 1, \cdots, 9\}$



Predict Articles' Topics (Multi-label)

$y = (\text{religion, politics, science})$

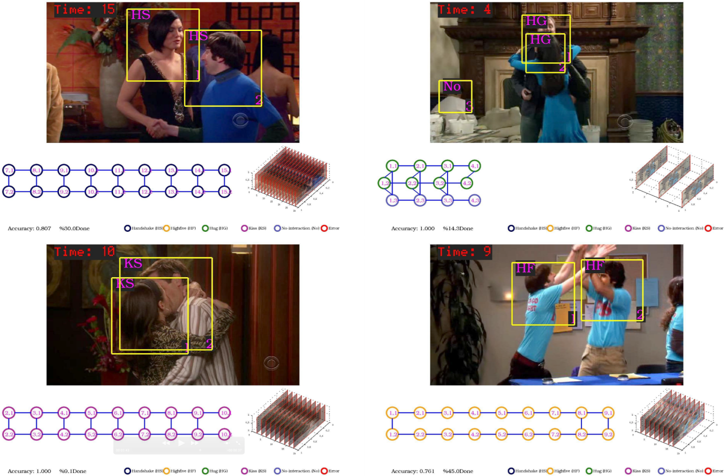
article	religion	politics	science
1	No	Yes	Yes
2	No	No	Yes
3	Yes	No	No
...			

Automatic Paragraph Segmentation (structured output)

"I'm afraid," said Holmes, smiling, "that all the queen's horses and all the queen's men cannot avail in this matter." 0
He had spread out his big map of London and leaned eagerly over it.
"Well, well," said he presently with an exclamation of satisfaction, "things are turning a little in our direction at last.
Why, Watson, I do honestly believe that we are going to pull it off, after all."
He slapped me on the shoulder with a sudden burst of hilarity.
"I am going out now.
It is only a reconnaissance.
I will do nothing serious without my trusted comrade and biographer at my elbow.
Do you stay here, and the odds are that you will see me again in an hour or two.
If time hangs heavy get foolscap and a pen, and begin your narrative of how we saved the State."
I felt some reflection of his elation in my own mind, for I knew well that he would not depart so far from his usual austerity of demeanour unless there was good cause for exultation. 10
All the long November evening I waited, filled with impatience for his return.
At last, shortly after nine o'clock, there arrived a messenger with a note:
Am dining at Goldini's Restaurant, Gloucester Road, Kensington. 13
Please come at once and join me there.
Bring with you a jemmy, a dark lantern, a chisel, and a revolver.
It was a nice equipment for a respectable citizen to carry through the dim, fog-draped streets. 16
I stowed them all discreetly away in my overcoat and drove straight to the address given.
There sat my friend at a little round table near the door of the garish Italian restaurant.
"Have you had something to eat? 19
Then join me in a coffee and curacao.
Try one of the proprietor's cigars. 130
They are less poisonous than one would expect.
Have you the tools?"

$y = (n_i)_{i=0}^{L-1}$,
n_i = beginning of paragraph i, L = number of boundaries
e.g. for this document $y = (0, 10, 13, 16, 19)$.

Human Interaction Recognition (structured output)



Novelty detection

Motivation: data from one class are easy to collect, and data from the rest class(es) are hard (or disastrous) to collect, or too few to be statistical meaningful.

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Example:

- Operational status of a nuclear plant as "normal"

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Motivation: data from one class are easy to collect, and data from the rest class(es) are hard (or disastrous) to collect, or too few to be statistical meaningful.

Example:

- Operational status of a nuclear plant as “normal”
- Seeing a baby elephant $\Rightarrow$ elephants are small?

Novelty detection

- Only "normal data" in your training dataset (thus seen all as 1-class).

Novelty detection

- Only "normal data" in your training dataset (thus seen all as 1-class).
- for a testing data point, to predict if it's "normal" (*i.e.* belong to that class or not).

Novelty detection

Q: Since belonging to one class or not, why not a binary classification problem?

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A: In novelty detection there are no "abnormal" data (*i.e.* 2nd class data) in the training dataset for you to train on.

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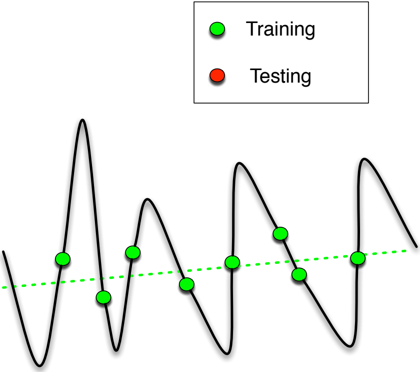
Q: Since belonging to one class or not, why not a binary classification problem?

A: In novelty detection there are no "abnormal" data (*i.e.* 2nd class data) in the training dataset for you to train on.

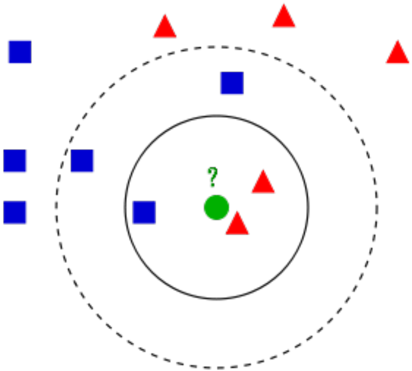
Other names: one-class classification, unary classification, outlier detection, anomaly detection

Regression

Continuous output y (to be covered in Lecture 4).



K Nearest Neighbour (KNN)



KNN: majority vote of the k Nearest Neighbours of the test point (green). If $k = 3$, the test point is predicted as red, if $k = 5$, the test point is predicted as blue. Picture courtesy of wikipedia

Questions

Thousands of classification algorithms out there. How can we possibly study they all?

Many algorithms come out every year, how do we keep up with them?

Answers

Learning theory analyses sets of algorithms' behaviour (will be covered in later lectures)

Many algorithms can be formulated in a unified framework called Empirical Risk Minimisation (ERM).

Risks

A typical $g(\mathbf{x}) = \text{sign}(\langle \mathbf{x}, \mathbf{w} \rangle)$, where $\text{sign}(z) = 1$ if $z > 0$, $\text{sign}(z) = -1$ otherwise. Given a loss $\ell(\mathbf{x}, y, \mathbf{w})$,

(True) Risk

$$R(\mathbf{w}, \ell) = \mathbb{E}_{(\mathbf{x},y)\sim p}\, \ell(\mathbf{x}, y, \mathbf{w})$$

Empirical Risk

$$R_n(\mathbf{w}, \ell) = \frac{1}{n} \sum_{i=1}^{n} \ell(\mathbf{x}_i, y_i, \mathbf{w})$$

The hinge loss

$\ell_H(\mathbf{x}, y, \mathbf{w}) = [1 - y(\langle \mathbf{x}, \mathbf{w} \rangle)]_+$, where $[z]_+ = \max\{0, z\}$.

The zero-one loss

$\ell_{0/1}(\mathbf{x}, y, \mathbf{w}) = \mathbf{1}_{g(\mathbf{x}) \neq y}$.

Generalisation error

Generalisation error is the error rate over all possible testing data from the distribution P, that is the risk w.r.t. zero loss,

$$R(g) = \mathbb{E}_{(\mathbf{x},y)\sim p}[\mathbf{1}_{g(\mathbf{x})\neq y}] = P(g(\mathbf{x}) \neq y)$$

(Zero-one) Empirical risk (training error)

$$R_n(g) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{g(\mathbf{x}_i)\neq y_i},$$

which is in fact the training error.

Regularised ERM

Regularised Empirical Risk Minimisation

$$g_n = \operatorname*{argmin}_{g \in \mathcal{G}} R_n(g) + \lambda \Omega(g),$$

where $\Omega(g)$ is the regulariser, *e.g.* $\Omega(g) = \|g\|^2$. $\mathcal{G}$ is the hypothesis set. Unfortunately, above is not convex. It turns out that one can optimise

$$\mathbf{w}_n = \operatorname*{argmin}_{\mathbf{w} \in \mathcal{W}} R_n(\mathbf{w}, \ell) + \lambda \Omega(\mathbf{w}),$$

as long as ℓ is a surrogate loss (brief def here) of the zero-one loss.

Decision functions

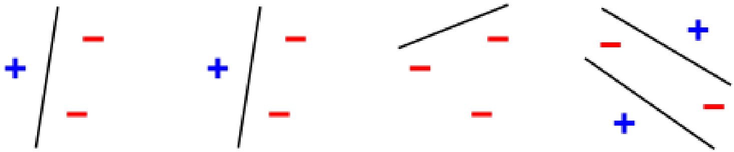
Linear decision function $g(\mathbf{x}; \mathbf{w}) = \text{sign}(\langle \mathbf{x}, \mathbf{w} \rangle + b)$ are often used (sign here is for binary classification). Here $\mathbf{x}, \mathbf{w} \in \mathbb{R}^d$, $b \in \mathbb{R}$. Since $\langle \mathbf{x}, \mathbf{w} \rangle + b = \langle [\mathbf{x}; 1], [\mathbf{w}; b] \rangle$, for simplicity one often write

Binary $\quad g(\mathbf{x}; \mathbf{w}) = \text{sign}(\langle \mathbf{x}, \mathbf{w} \rangle).$

Multi-class $\quad g(\mathbf{x}; \mathbf{w}) = \underset{y}{\text{argmax}}(\langle \mathbf{x}, \mathbf{w}_y \rangle).$

Separability

Not all data are linearly separable (*e.g.* the 4-th one).



Picture courtesy of wikipedia

To deal with linearly non-separable case, non-linear decision functions are needed (often used in kernel methods).

Perceptron

Assume $g(\mathbf{x}; \mathbf{w}) = \text{sign}(\langle \mathbf{x}, \mathbf{w} \rangle)$, where $\mathbf{x}, \mathbf{w} \in \mathbb{R}^d$. $y \in \{-1, 1\}$

Input: training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, step size η, #iter T
Initialise $w_1 = \mathbf{0}$
for $t = 1$ **to** T **do**

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \eta \sum_{i=1}^{n} (y_i \, \mathbf{x}_i \, \mathbf{1}_{y_i \langle \mathbf{x}_i, \mathbf{w}_t \rangle < 0}) \tag{1}$$

end for
Output: $\mathbf{w}^* = \mathbf{w}_T$

The class of $\mathbf{x}$ is predicted via

$$y^* = \text{sign}(\langle \mathbf{x}, \mathbf{w}^* \rangle)$$

View it in ERM

$$\min_{\mathbf{w},\xi} \frac{1}{n}\sum_{i=1}^{n}\xi_i, \quad \text{s.t.} \quad y_i \langle \mathbf{x}_i, \mathbf{w}\rangle \geq -\xi_i, \xi_i \geq 0$$

whose unconstrained form is

$$\min_{\mathbf{w}} \frac{1}{n}\sum_{i=1}^{n}[-y_i \langle \mathbf{x}_i, \mathbf{w}\rangle]_+ \Leftrightarrow \min_{\mathbf{w}} R_n(\mathbf{w}, \ell_{pern})$$

with Loss $\ell_{pern}(\mathbf{x}, y, \mathbf{w}) = [-y \langle \mathbf{x}, \mathbf{w}\rangle]_+$ and
Empirical Risk $R_n(\mathbf{w}, \ell_{pern}) = \frac{1}{n}\sum_{i=1}^{n} \ell_{pern}(\mathbf{x}_i, y_i, \mathbf{w})$.

Sub-gradient $$\frac{\partial R_n(\mathbf{w}, \ell_{pern})}{\partial \mathbf{w}} = -\frac{1}{n}\sum_{i=1}^{n}(y_i\, \mathbf{x}_i\, \mathbf{1}_{y_i(\langle \mathbf{x}_i, \mathbf{w}_t\rangle)<0}).$$

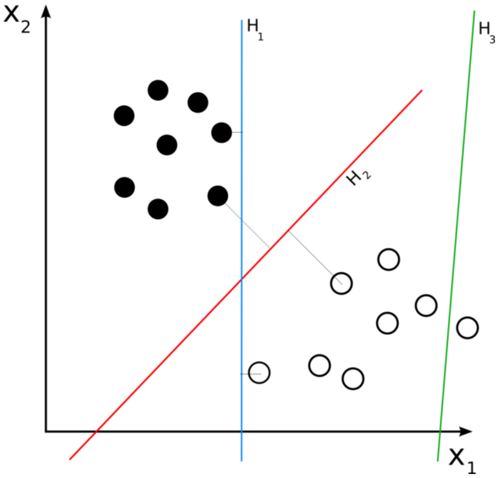
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta' \frac{\partial R_n(\mathbf{w}, \ell_{pern})}{\partial \mathbf{w}} = \mathbf{w}_t + \eta' \frac{1}{n}\sum_{i=1}^{n}(y_i\, \mathbf{x}_i\, \mathbf{1}_{y_i(\langle \mathbf{x}_i, \mathbf{w}_t\rangle)<0})$$

Letting $\eta = \eta' \frac{1}{n}$ recovers the equation (1).

Break

Take a break ...

Max Margin



Max Margin Formulation

One form of soft margin binary Support Vector Machines (SVMs) (a primal form) is

$$\min_{\mathbf{w},b,\gamma,\xi} -\gamma + C\sum_{i=1}^{n}\xi_i \tag{2}$$
$$\text{s.t. } y_i(\langle \mathbf{x}_i, \mathbf{w}\rangle + b) \geq \gamma - \xi_i, \xi_i \geq 0, \| \mathbf{w} \|^2 = 1$$

For a testing $\mathbf{x}'$, given the learnt $\mathbf{w}^*$, b^*, the predicted label

$y^* = g(\mathbf{x}'; \mathbf{w}^*) = \text{sign}(\langle \mathbf{x}', \mathbf{w}^* \rangle + b^*)$.

Primal

A more popular version is (still a primal form)

$$\min_{\mathbf{w},b,\xi} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n} \xi_i,$$

$$\text{s.t.} \quad y_i(\langle \mathbf{x}_i, \mathbf{w}\rangle + b) \geq 1 - \xi_i, \xi_i \geq 0, i = 1, \cdots, n,$$

This is equivalent to the previous form and $\gamma = 1/\|\mathbf{w}\|$.

In ERM, it corresponds to
The hinge loss $\ell_H(\mathbf{x}, y, \mathbf{w}) = [1 - y(\langle \mathbf{x}, \mathbf{w}\rangle + b)]_+$, and
$\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2$ with a proper λ.

Recall duality

For a convex minimisatin problem (*i.e.* f_0, f_i are convex)

$$\min_{\mathbf{x}} f_0(\mathbf{x})$$
$$\text{s.t.} \quad f_i(\mathbf{x}) \leq 0, i = 1, \cdots, m,$$

the Lagrangian dual problem is

$$\max_{\alpha} D(\alpha)$$
$$\text{s.t.} \quad \alpha_i \geq 0, i = 1, \cdots, m,$$

where $D(\alpha) := \inf_{\mathbf{x}}\{L(\mathbf{x}, \alpha)\}$, and the Lagrange function $L(\mathbf{x}, \alpha) = f_0(\mathbf{x}) + \sum_{i=1}^{m} \alpha_i f_i(\mathbf{x})$.

Recall duality

The following always holds
$D(\alpha) \leq f_0(\mathbf{x}), \; \forall \mathbf{x}, \alpha$ (so called weak duality)

Sometimes (not always) below holds
$\max_\alpha D(\alpha) = \min_\mathbf{x} f_0(\mathbf{x})$ (so called strong duality)
Strong duality holds for SVM.

Lagrangian function

$$L(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{1}{2} \| \mathbf{w} \|^2 + C \sum_{i=1}^{n} \xi_i$$
$$+ \sum_{i=1}^{n} \alpha_i [1 - \xi_i - y_i(\langle \mathbf{x}_i, \mathbf{w} \rangle + b)] + \sum_{i=1}^{n} \beta_i(-\xi_i)$$

Optimise Lagrangian function — 1st order condition

To get $\inf_{\mathbf{w},b,\xi}\{L(\mathbf{w},b,\xi,\alpha,\beta)\}$, by 1st order condition

$$\frac{\partial L(\mathbf{w},b,\xi,\alpha,\beta)}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w}^* - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \tag{3}$$

$$\frac{\partial L(\mathbf{w},b,\xi,\alpha,\beta)}{\partial \xi_i} = 0 \Rightarrow C - \alpha_i - \beta_i = 0 \tag{4}$$

$$\frac{\partial L(\mathbf{w},b,\xi,\alpha,\beta)}{\partial b} = 0 \Rightarrow \sum_{i=1}^{n} \alpha_i y_i = 0 \tag{5}$$

Optimise Lagrangian function — Complementarity conditions

Complementarity conditions

$$\alpha_i[1 - \xi_i - y_i(\langle \mathbf{x}_i, \mathbf{w} \rangle + b)] = 0, \forall i \tag{6}$$

$$\beta_i \xi_i = 0, \forall i \tag{7}$$

Dual

$$
\begin{aligned}
& L(\mathbf{w}^*, b^*, \xi^*, \alpha, \beta) \\
&= \frac{1}{2}\langle \mathbf{w}^*, \mathbf{w}^* \rangle + \sum_{i=1}^n \alpha_i - \sum_{i=1}^n \alpha_i y_i \langle \mathbf{x}_i, \mathbf{w}^* \rangle \\
&+ \sum_{i=1}^n \xi_i^* (C - \alpha_i - \beta_i) + b(\sum_{i=1}^n \alpha_i y_i) \\
&= \frac{1}{2}\langle \mathbf{w}^*, \mathbf{w}^* \rangle + \sum_{i=1}^n \alpha_i - \sum_{i=1}^n \alpha_i y_i \langle \mathbf{x}_i, \mathbf{w}^* \rangle \quad \text{via eq(4) and eq(5)} \\
&= \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle + \sum_{i=1}^n \alpha_i - \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle \ \text{ via eq(3)} \\
&= \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle
\end{aligned}
$$

Dual

$\max_\alpha \inf_{\mathbf{w},b,\xi}\{L(\mathbf{w},b,\xi,\alpha,\beta)\}$ gives the dual form:

$$\max_\alpha \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i\alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$
$$\text{s.t.} \quad 0 \leq \alpha_i \leq C, i = 1, \cdots, n, \quad \text{(via eq(4))}$$

Let α^* be the solution.

From dual to primal variables

How to compute $\mathbf{w}^*, b^*$ from α^*?
Via eq(3), we have

$$\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i. \tag{8}$$

Via comp condition eq(6), we have $\alpha_i[1 - \xi_i - y_i(\langle \mathbf{x}_i, \mathbf{w} \rangle + b)] = 0, \forall i$. When $\alpha_i > 0$, we know $1 - \xi_i - y_i(\langle \mathbf{x}_i, \mathbf{w} \rangle + b) = 0$. It will be great if $\xi_i = 0$ too. When will it happen? $\beta_i > 0 \Rightarrow \xi_i$ because of comp condition eq(7). Since $C - \alpha_i - \beta_i = 0$ (4), $\beta_i > 0$ means $\alpha < C$.
For any i, s.t. $0 < \alpha_i < C$, $1 - y_i(\langle \mathbf{x}_i, \mathbf{w} \rangle + b) = 0$, so (multiple y_i on both sides, and the fact that $y_i^2 = 1$)

$$b^* = y_i - \langle \mathbf{x}_i, \mathbf{w}^* \rangle \tag{9}$$

Numerically wiser to take the average over all such training points (Burges tutorial).

Support Vectors

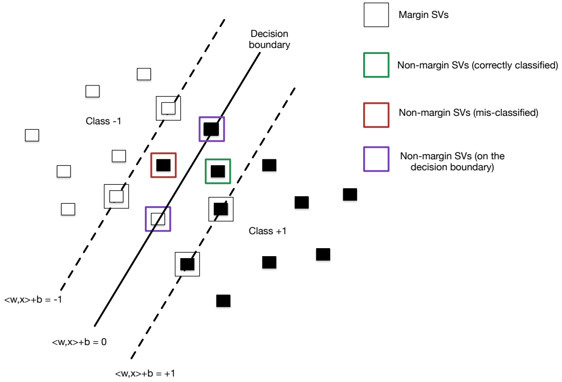
$y^* = \text{sign}(\langle x, \mathbf{w}^* \rangle + b^*) = \text{sign}(\sum_{i=1}^{n} \alpha_i^* y_i \langle \mathbf{x}_i, x \rangle + b^*)$.

It turns out many $\alpha_i^* = 0$. Those $\mathbf{x}_j$ with $\alpha_j^* > 0$ are called support vectors. Let $S = \{j : \alpha_j^* > 0\}$

$$y^* = \text{sign}(\sum_{j \in S} \alpha_j^* y_j \langle \mathbf{x}_j, \mathbf{x} \rangle + b^*)$$

Note now y can be predicted without explicitly expressing $\mathbf{w}$ as long as the support vectors are stored.

Support Vectors



Two types of SVs:

- Margin SVs: $0 < \alpha_i < C$ ($\xi_i = 0$, on the dash lines)
- Non-margin SVs: $\alpha_i = C$ ($\xi_i > 0$, thus violating the margin. More specifically, when $1 > \xi_i > 0$, correctly classified; when $\xi_i > 1$, it's mis-classified; when $\xi_i = 1$, on the decision boundary)

Dual

All derivation holds if one replaces $\mathbf{x}_j$ with $\phi(\mathbf{x}_j)$ and let kernel function $\kappa(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$. This gives

$$
\begin{aligned}
&\max_{\alpha} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \\
&\text{s.t.} \quad 0 \le \alpha_i \le C, i = 1, \cdots, n
\end{aligned}
$$

$$
y^* = \text{sign}[\sum_{j \in S} \alpha_j^* y_j \kappa(\mathbf{x}_j, \mathbf{x}) + b^*].
$$

This leads to non-linear SVM and more generally kernel methods (will be covered in later lectures).

Theoretical justification

An example of generalisation bounds is below.

Theorem (VC bound)

Denote h as the VC dimension, for all $n \geq h$, for any $\delta \in (0,1)$, with probability at least $1-\delta$, $\forall g \in \mathcal{G}$

$$R(g) \leq R_n(g) + 2\sqrt{2\frac{h\log\frac{2en}{h} + \log(\frac{2}{\delta})}{n}}.$$

Margin $\gamma = 1/\|\mathbf{w}\|$, $h \leq \min\{D, \lceil\frac{4R^2}{\gamma^2}\rceil\}$, where the radius $R^2 = \max_{i=1}^{n}\langle\Phi(\mathbf{x}_i), \Phi(\mathbf{x}_i)\rangle$ (assuming data are already centered)

Theoretical justification

Other tighter bounds such as Rademacher bounds, PAC-Bayes bounds *etc.* (Generalisation bounds will be covered in later lectures).

Logistic Regression for Binary Classification

For binary LR, one can assume

$$P(y = +1|\,\mathbf{x};\mathbf{w}) = \frac{1}{1 + e^{-\langle \mathbf{w},\mathbf{x}\rangle}}$$

Thus

$$\begin{aligned} P(y = -1|\,\mathbf{x};\mathbf{w}) &= 1 - P(y = +1|\,\mathbf{x};\mathbf{w}) \\ &= \frac{e^{-\langle \mathbf{w},\mathbf{x}\rangle}}{1 + e^{-\langle \mathbf{w},\mathbf{x}\rangle}} = \frac{1}{1 + e^{\langle \mathbf{w},\mathbf{x}\rangle}} \end{aligned}$$

Above means

$$P(y|\,\mathbf{x};\mathbf{w}) = \frac{1}{1 + e^{-y\langle \mathbf{w},\mathbf{x}\rangle}} \tag{10}$$

Alternative formulation

Alternatively if let $y \in \{0, 1\}$, one assumes

$$P(y = +1|\,\mathbf{x}; \mathbf{w}) = \frac{1}{1 + e^{-\langle \mathbf{w}, \mathbf{x} \rangle}}$$
$$P(y = 0|\,\mathbf{x}; \mathbf{w}) = \frac{1}{1 + e^{\langle \mathbf{w}, \mathbf{x} \rangle}},$$

which means

$$P(y|\,\mathbf{x}; \mathbf{w}) = \left(\frac{1}{1 + e^{-\langle \mathbf{w}, \mathbf{x} \rangle}}\right)^{y} \left(\frac{1}{1 + e^{\langle \mathbf{w}, \mathbf{x} \rangle}}\right)^{(1-y)} \tag{11}$$

Because eq(11) is not as neat as eq(10), we will use eq(10) with $y \in \{-1, 1\}$.

Maximum Likelihood and Log loss

Maximum Likelihood

$$\operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{n} P(y_i | \mathbf{x}_i; \mathbf{w})$$

$$= \operatorname*{argmin}_{\mathbf{w}} -\log\left(\prod_{i=1}^{n} P(y_i | \mathbf{x}_i; \mathbf{w})\right)$$

$$= \operatorname*{argmin}_{\mathbf{w}} -\sum_{i=1}^{n} \log P(y_i | \mathbf{x}_i; \mathbf{w}) \quad \text{(log loss in ERM)}$$

Gradient for binary

Let

$$L(\mathbf{w}\,|X, Y) = -\sum_{i=1}^{n} \log P(y_i |\, \mathbf{x}_i; \mathbf{w})$$

$$\frac{\partial L(\mathbf{w}\,|X, Y)}{\partial\, \mathbf{w}} = \frac{\partial \sum_{i=1}^{n} \log \left(1 + e^{-y_i \langle \mathbf{w}, \mathbf{x}_i \rangle}\right)}{\partial\, \mathbf{w}} \quad \text{via eq(10)}$$

$$= \sum_{i=1}^{n} \frac{e^{-y_i \langle \mathbf{w}, \mathbf{x}_i \rangle}}{1 + e^{-y_i \langle \mathbf{w}, \mathbf{x}_i \rangle}} (-y_i\, \mathbf{x}_i)$$

$$= \sum_{i=1}^{n} (-y_i\, \mathbf{x}_i)(1 - P(y_i |\, \mathbf{x}_i; \mathbf{w}))$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\partial L(\mathbf{w}\,|X, Y)}{\partial\, \mathbf{w}}$$

Multi-class

For multi-class LR, let c be the number of classes. Let $\mathbf{w} = (\mathbf{w}_{y'})_{y' \in \mathcal{Y}}$, where $\mathbf{w}_{y'} \in \mathbb{R}^d$, thus $\mathbf{w} \in \mathbb{R}^{dc}$. One assumes

$$P(y|\,\mathbf{x};\mathbf{w}) = \frac{e^{\langle \mathbf{w}_y, \mathbf{x} \rangle}}{\sum_{y' \in \mathcal{Y}} e^{\langle \mathbf{w}_{y'}, \mathbf{x} \rangle}} \tag{12}$$

Note: the multi-class form can recover the binary form despite different appearance.

$$\begin{aligned} L(\mathbf{w}\,|X, Y) &= -\sum_{i=1}^{n} \log P(y_i|\,\mathbf{x}_i;\mathbf{w}) \\ &= \sum_{i=1}^{n} \log(\sum_{y' \in \mathcal{Y}} e^{\langle \mathbf{w}_{y'}, \mathbf{x}_i \rangle}) - \langle \mathbf{w}_y, \mathbf{x}_i \rangle \end{aligned}$$

Gradient for Multi-class

$$\frac{\partial L(\mathbf{w} \,|X, Y)}{\partial \, \mathbf{w}_y} = \sum_{i=1}^{n} \Big(\frac{e^{\langle \mathbf{w}_y, \mathbf{x}_i \rangle}}{\sum_{y' \in \mathcal{Y}} e^{\langle \mathbf{w}_{y'}, \mathbf{x}_i \rangle}} \, \mathbf{x}_i - \mathbf{x}_i \Big)$$

$$= \sum_{i=1}^{n} \mathbf{x}_i (P(y_i | \, \mathbf{x}_i; \mathbf{w}) - 1)$$

$$\frac{\partial L(\mathbf{w} \,|X, Y)}{\partial \, \mathbf{w}} = \Big(\frac{\partial L(\mathbf{w} \,|X, Y)}{\partial \, \mathbf{w}_y} \Big)_{y \in \mathcal{Y}}$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\partial L(\mathbf{w} \,|X, Y)}{\partial \, \mathbf{w}}$$

Supervised Learning definition revisit

Definition (Lecture 1)

Given input-output data pairs $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ sampled from an unknown but fixed distribution $p(\mathbf{x}, y)$, the goal is to learn $g : \mathcal{X} \to \mathcal{Y}$, $g \in \mathcal{G}$ s.t. $p(g(\mathbf{x}) \neq y)$ is small.

$p(g(\mathbf{x}) \neq y)$ is mainly for classification, not very suitable for regression.

Supervised Learning definition revisit

A more general definition for SL (than the previous lecture):

Definition (revisit)

Given input-output data pairs $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ sampled from an unknown but fixed distribution $p(\mathbf{x}, y)$, the goal is to learn $g : \mathcal{X} \to \mathcal{Y}$, $g \in \mathcal{G}$ s.t. $\cancel{p(g(\mathbf{x}) \neq y)}$ the risk $\mathbb{E}_{(\mathbf{x},y)\sim p}[\ell(g(\mathbf{x}), y)]$ is small w.r.t. certain loss ℓ.

$\mathbb{E}_{(\mathbf{x},y)\sim p}[\ell(g(\mathbf{x}), y)]$ is more general (applicable to classification, and regression).

Extension to structured output

SVMs are extended to what known as Structured SVM.

Logistic Regression is extended to what later known as Conditional Random Fields.

Structured case will be covered in later lectures.

That's all

Thanks!