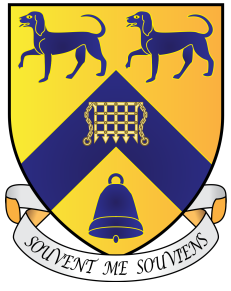
# Statistical (Supervised) Learning Theory

## FoPSS Logic and Learning School



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# Previous Mini-Course

Introduction to Computational Learning Theory (PAC)

Learnability and the VC dimension

Sample Compression Schemes

Learning with Membership Queries

(Computational) Hardness of Learning

# This Mini-Course

Statistical Learning Theory Framework

Capacity Measures : Rademacher Complexity

Uniform Convergence : Generalisation Bounds

Some Machine Learning Techniques

Algorithmic Stability to prove Generalisation

# Outline

Statistical (Supervised) Learning Theory Framework

Linear Regression

Rademacher Complexity

Support Vector Machines

Kernels

Neural Networks

Algorithmic Stability

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Sometimes convenient to factorise: $D(\mathbf{x}, y) = D(\mathbf{x})D(y|\mathbf{x})$

Make no assumptions about a specific functional relationship between $\mathbf{x}$ and $y$, a.k.a. agnostic setting [10,13,16]

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We will focus on fitting functions from a class of functions whose "complexity" or "capacity" is bounded

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Attempt to explicitly model the distributions $D(\mathbf{x})$ and/or $D(y|\mathbf{x})$

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- Classification: $y|w_0, \mathbf{w}, \mathbf{x} \sim 2 \cdot \text{Bernoulli}(\text{sigmoid}(w_0 + \mathbf{w} \cdot \mathbf{x})) - 1$

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The (basic) PAC model in CLT assumes a functional form, $y = c(\mathbf{x})$, for some concept $c$ in class $C$, and the VC dimension of $C$ controls learnability.

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A cost function $\gamma : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$

- E.g. $\mathcal{Y} = \{-1, 1\}$, $\gamma(y', y) = \mathbb{I}(y' \neq y)$
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Goal: To guarantee with high probability (over $S$) that if $\widehat{f} = A(S)$, then for some small $\epsilon > 0$:

$$R(\widehat{f}) \leq \inf_{f\in\mathcal{F}} R(f) + \epsilon$$

# Empirical Risk Minimisation

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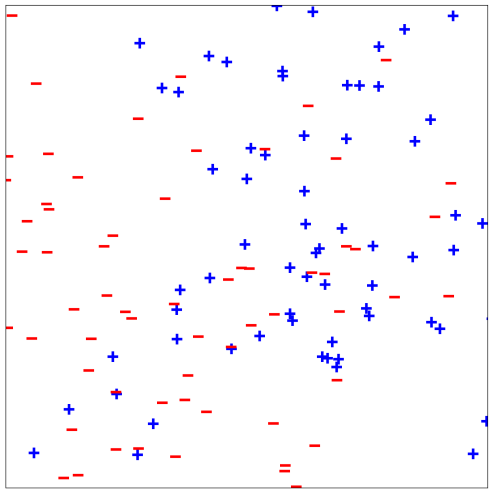

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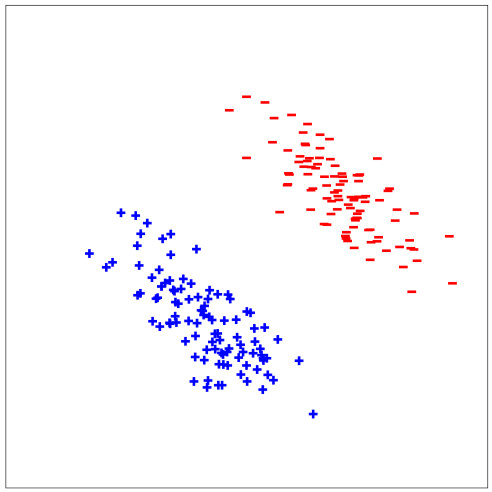

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Let $\mathcal{F} \subset \{-1, 1\}^{\mathcal{X}}$ with $\text{VC}(\mathcal{F}) = d < \infty$. Let $S \sim D^m$ for some distribution $D$ over $\mathcal{X} \times \{-1, 1\}$. Then, for every $\delta > 0$, with probability at least $1 - \delta$, for every $f \in \mathcal{F}$,

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Where $\epsilon$ is chosen to be a suitable function of $\delta$ and $m$

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Choose an infinite family of classes $\{\mathcal{F}_d : d = 1, 2, \ldots\}$ and find the minimiser:

$$\widehat{f} = \operatorname*{argmin}_{f \in \mathcal{F}_d, d \in \mathbb{N}} \widehat{R}_S(f) + \kappa(d, m)$$

where $\kappa(d, m)$ is a penalty term that depends on the sample size and the "complexity" or "capacity" measure

# Structural Risk Minimisation

$$R(f) \leq \widehat{R}_S(f) + \sqrt{\frac{2d\log(em/d)}{m}} + O\left(\sqrt{\frac{\log(1/\delta)}{2m}}\right)$$

How should be pick the class of functions $\mathcal{F}$?

- More "complex" $\mathcal{F}$ can achieve smaller empirical risk
- Difference between true risk and empirical risk (generalisation error) will be higher for more "complex" $\mathcal{F}$

Choose an infinite family of classes $\{\mathcal{F}_d : d = 1, 2, \ldots\}$ and find the minimiser:

$$\widehat{f} = \operatorname*{argmin}_{f \in \mathcal{F}_d, d \in \mathbb{N}} \widehat{R}_S(f) + \kappa(d, m)$$

where $\kappa(d, m)$ is a penalty term that depends on the sample size and the "complexity" or "capacity" measure

Related to the more commonly used approach in practice:

$$\widehat{f} = \operatorname*{argmin}_{f \in \mathcal{F}} \widehat{R}_S(f) + \lambda \cdot \text{regulariser}(f)$$

# Outline

Statistical (Supervised) Learning Theory Framework

Linear Regression

Rademacher Complexity

Support Vector Machines

Kernels

Neural Networks

Algorithmic Stability

# Linear Regression

Let $K \subset \mathbb{R}^n$. Consider the family of linear functions

$$\mathcal{F} = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \mid \mathbf{w} \in K\}$$

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$$R(h) = \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim D}\left[(h(\mathbf{x}) - y)^2\right] = \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim D}\left[(h(\mathbf{x}) - g(\mathbf{x}) + g(\mathbf{x}) - y)^2\right]$$

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If $g \in \mathcal{F}$, we are in the so-called realisable setting

# Aside: Maximum Likelihood Principle

Discriminative Setting: Model $y \mid \mathbf{w}, \mathbf{x} \sim \mathbf{w} \cdot \mathbf{x} + \mathcal{N}(0, \sigma^2)$

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We can defined the likelihood of observing the data under this model

$$p(y_1, \ldots, y_m \mid \mathbf{w}, \mathbf{x}_1, \ldots, \mathbf{x}_m) = \frac{1}{(2\pi\sigma^2)^{m/2}} \prod_{i=1}^{m} \exp\left(-\frac{(y_i - \mathbf{w} \cdot \mathbf{x}_i)^2}{2\sigma^2}\right)$$

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Finding parameters $\mathbf{w}$ that maximise the (log) likelihood is the same as finding $\mathbf{w}$ that minimises the empirical risk with the squared error cost

The method of least squares goes back at least 200 years to Gauss, Laplace

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We will require some boundedness assumptions on the data and the linear functions

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Then the Empirical Rademacher Complexity of $\mathcal{G}$ with respect to $S$ is defined as:

$$\widehat{\mathfrak{R}}_S(\mathcal{G}) = \mathop{\mathbb{E}}_{\boldsymbol{\sigma} \sim_u \{-1,1\}^m} \left[ \sup_{g \in \mathcal{G}} \frac{1}{m} \sum_{i=1}^{m} \sigma_i g(z_i) \right]$$

where $(\sigma_1, \ldots, \sigma_m) =: \boldsymbol{\sigma} \sim_u \{-1, 1\}^m$ indicates that each $\sigma_i$ is a random variable taking the values $\{-1, 1\}$ with equal probability. These are called Rademacher random variables

# Rademacher Complexity

**Empirical Rademacher Complexity**

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## Rademacher Complexity

Let $D$ be a distribution over the set $\mathcal{Z}$. Let $\mathcal{G}$ be a class of functions from $\mathcal{Z} \to [a, b] \subset \mathbb{R}$. For any $m \geq 1$, the Rademacher complexity of $\mathcal{G}$ is the expectation of the empirical Rademacher complexity of $\mathcal{G}$ over a sample drawn from $D^m$:

$$\mathfrak{R}_m(\mathcal{G}) = \mathop{\mathbb{E}}_{S \sim D^m} \left[ \widehat{\mathfrak{R}}_S(\mathcal{G}) \right]$$

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## Theorem [2,14]

Let $\mathcal{G}$ be a class of functions mapping $\mathcal{Z} \to [0,1]$. Let $D$ be a distribution over $\mathcal{Z}$ and suppose that a sample $S$ of size $m$ is drawn from $D^m$. Then for every $\delta > 0$, with probability at least $1-\delta$, the following holds for each $g \in \mathcal{G}$:

$$\mathop{\mathbb{E}}_{z\sim D}\left[g(z)\right] \leq \frac{1}{m}\sum_{i=1}^{m} g(z_i) + 2\mathfrak{R}_m(\mathcal{G}) + O\left(\sqrt{\frac{\log(1/\delta)}{m}}\right).$$

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Henceforth, for $S = \{z_1, \ldots, z_m\}$, we will use the notation:

$$\mathop{\widehat{\mathbb{E}}}_{z\sim_u S}\left[g(z)\right] = \frac{1}{m}\sum_{i=1}^m g(z_i)$$

We will see a full proof of this theorem. First, let's apply this to linear regression.

# Generalisation Bounds for Linear Regression

Instance space $\mathcal{X} \subset \mathbb{R}^n$, $\forall \mathbf{x} \in \mathcal{X}, \|\mathbf{x}\|_2 \leq X$

Target values $\mathcal{Y} = [-M, M]$

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$$\begin{aligned}
\widehat{\mathfrak{R}}_S(\mathcal{F}) &= \frac{1}{m}\mathop{\mathbb{E}}_{\boldsymbol{\sigma}}\left[\sup_{\mathbf{w}, \|\mathbf{w}\|_2 \leq W} \sum_{i=1}^{m} \sigma_i(\mathbf{w} \cdot \mathbf{x}_i)\right] \\
&= \frac{1}{m}\mathop{\mathbb{E}}_{\boldsymbol{\sigma}}\left[\sup_{\mathbf{w}, \|\mathbf{w}\|_2 \leq W} \mathbf{w} \cdot \sum_{i=1}^{m} \sigma_i \mathbf{x}_i\right] \\
&= \frac{W}{m}\mathop{\mathbb{E}}_{\boldsymbol{\sigma}}\left[\left\|\sum_{i=1}^{m} \sigma_i \mathbf{x}_i\right\|_2\right]
\end{aligned}$$

The last step follows from (the equality condition of) the Cauchy-Schwartz Inequality

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$$= \frac{W}{m}\left(\mathop{\mathbb{E}}_{\boldsymbol{\sigma}}\left[\sum_{i=1}^{m}\sigma_i^2\|\mathbf{x}_i\|_2^2 + \underbrace{2\sum_{i<j}\sigma_i\sigma_j\mathbf{x}_i\cdot\mathbf{x}_j}_{=0 \text{ as } \sigma_i \text{ are independent}}\right]\right)^{\frac{1}{2}}$$

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$$= \frac{W}{m}\left(\mathop{\mathbb{E}}_{\boldsymbol{\sigma}}\left[\sum_{i=1}^m \sigma_i^2 \|\mathbf{x}_i\|_2^2 + \underbrace{2\sum_{i<j} \sigma_i \sigma_j \mathbf{x}_i \cdot \mathbf{x}_j}_{=0 \text{ as } \sigma_i \text{ are independent}}\right]\right)^{\frac{1}{2}}$$

$$= \frac{W}{m}\left(\sum_{i=1}^m \|\mathbf{x}_i\|_2^2\right)^{\frac{1}{2}} = \frac{WX}{\sqrt{m}}$$

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Then Talagrand's Lemma tells us that:

$$\widehat{\mathfrak{R}}_S(\phi \circ \mathcal{G}) \leq L \cdot \widehat{\mathfrak{R}}_S(\mathcal{G})$$
$$\mathfrak{R}_m(\phi \circ \mathcal{G}) \leq L \cdot \mathfrak{R}_m(\mathcal{G})$$

# Generalisation of Linear Regression

Instance space $\mathcal{X} \subset \mathbb{R}^n$, $\forall \mathbf{x} \in \mathcal{X}, \|\mathbf{x}\|_2 \leq X$

Target values $\mathcal{Y} = [-M, M]$

Let $\mathcal{F} = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \mid \|\mathbf{w}\|_2 \leq W\}$

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Consider the following:

$$\mathcal{H} = \{(\mathbf{x}, y) \mapsto (f(\mathbf{x}) - y)^2 \mid \mathbf{x} \in \mathcal{X}, y \in \mathcal{Y}, f \in \mathcal{F}\}$$

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Note that $\mathfrak{R}_m(\mathcal{H}) = \mathop{\mathbb{E}}_{S \sim D^m}\left[\widehat{\mathfrak{R}}_S(\mathcal{H})\right] \leq \sup_{S, |S|=m} \widehat{\mathfrak{R}}_S(\mathcal{H})$

# Aside: Algorithms for the Linear Regression Model

## ERM for Linear Regression

$$J(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m}(\mathbf{w}\cdot\mathbf{x}_i - y_i)^2$$

$$\widehat{\mathbf{w}} = \operatorname*{argmin}_{\mathbf{w},\|\mathbf{w}\|_2\leq W} J(\mathbf{w})$$

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This convex optimisation problem can be solved using projected (stochastic) gradient descent

Guaranteed to find a near-optimal solution in polynomial time

# Aside: Gradient Descent

**Algorithm** Projected Gradient Descent

**Inputs**: $\eta, T$

Pick $\mathbf{w}_1 \in K$

**for** $t = 1, \ldots, T$ **do**

$\mathbf{w}'_{t+1} = \mathbf{w}_t - \eta \nabla J(\mathbf{w}_t)$

$\mathbf{w}_{t+1} = \Pi_K(\mathbf{w}'_{t+1})$

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**Informal Theorem** [5]

Suppose $\sup_{\mathbf{w},\mathbf{w}' \in K} \left\|\mathbf{w} - \mathbf{w}'\right\|_2 \leq R$ and $\sum_{\mathbf{w} \in K} \left\|\nabla J(\mathbf{w})\right\|_2 \leq L$, then with $\eta = R/(L\sqrt{T})$

$$J(\overline{\mathbf{w}}) \leq \min_{\mathbf{w} \in K} J(\mathbf{w}) + \frac{RL}{\sqrt{T}}$$

# Aside: Generalised Linear Models

Can consider more general models called generalised linear models

$$\text{GLM} = \{\mathbf{x} \mapsto u(\mathbf{w} \cdot \mathbf{x}) \mid u \text{ bounded, increasing \& } 1\text{-Lipschitz}, \|\mathbf{w}\|_2 \leq W\}$$

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Can bound Rademacher complexity easily using the boundedness and Lipschitz property of $u$

However, the optimisation problem is now non-convex!

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Can consider a different cost/loss function:

$$\gamma(y', y) = \int_0^{u^{-1}(y')} (u(z) - y)dz$$

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In the realisable setting, i.e. $\mathbb{E}\left[y \,|\mathbf{x}\right] = u(\mathbf{w} \cdot \mathbf{x})$, the global minimisers of $J(\mathbf{w})$ (squared error) and $\widetilde{J}(\mathbf{w})$ coincide, yielding computationally and statistically efficient algorithms. [12]

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**Theorem** [2,14]

Let $\mathcal{G}$ be a class of functions mapping $\mathcal{Z} \to [0,1]$. Let $D$ be a distribution over $\mathcal{Z}$ and suppose that a sample $S$ of size $m$ is drawn from $D^m$. Then for every $\delta > 0$, with probability at least $1 - \delta$, the following holds for each $g \in \mathcal{G}$:

$$\mathop{\mathbb{E}}_{z \sim D}\left[g(z)\right] \leq \frac{1}{m}\sum_{i=1}^{m} g(z_i) + 2\mathfrak{R}_m(\mathcal{G}) + O\left(\sqrt{\frac{\log(1/\delta)}{m}}\right).$$

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We will make use of a concentration of measure inequality, called McDiarmid's inequality.

## McDiarmid's Inequality

Let $\mathcal{Z}$ be a set and let $f : \mathcal{Z}^m \to \mathbb{R}$ be a function such that, $\forall i, \exists c_i > 0, \forall z_1, \ldots, z_m, z_i'$,

$$|f(z_1, \ldots, z_i, \ldots, z_m) - f(z_1, \ldots, z_i', \ldots, z_m)| \leq c_i.$$

Let $Z_1, \ldots, Z_m$ be i.i.d. random variables taking values in $\mathcal{Z}$, then $\forall \varepsilon > 0$,

$$\mathbb{P}\left[f(Z_1, \ldots, Z_m) \geq \mathbb{E}\left[f(Z_1, \ldots, Z_m)\right] + \varepsilon\right] \leq \exp\left(-\frac{2\varepsilon^2}{\sum_i c_i^2}\right)$$

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**Want to show**

$$\mathop{\mathbb{E}}_{z \sim D} \left[ g(z) \right] \leq \frac{1}{m} \sum_{i=1}^{m} g(z_i) + 2\mathfrak{R}_m(\mathcal{G}) + O\left( \sqrt{\frac{\log(1/\delta)}{m}} \right).$$

# Proof of Main Result

$$\Phi(S) = \sup_{g \in \mathcal{G}} \left( \mathop{\mathbb{E}}_{z \sim D} \left[ g(z) \right] - \mathop{\widehat{\mathbb{E}}}_{z \sim_u S} \left[ g(z) \right] \right)$$

Alternatively, for any $\delta > 0$, with probability at least $1 - \delta$,

$$\Phi(S) \leq \mathop{\mathbb{E}}_{S \sim D^m} \left[ \Phi(S) \right] + O\left( \sqrt{\frac{\log(1/\delta)}{m}} \right)$$

Thus, for any $\delta > 0$, with probability at least $1 - \delta$, for every $g \in \mathcal{G}$,

$$\mathop{\mathbb{E}}_{z \sim D} \left[ g(z) \right] \leq \mathop{\widehat{\mathbb{E}}}_{z \sim_u S} \left[ g(z) \right] + \mathop{\mathbb{E}}_{S \sim D^m} \left[ \Phi(S) \right] + O\left( \sqrt{\frac{\log(1/\delta)}{m}} \right)$$

Recall that,

$$\mathop{\widehat{\mathbb{E}}}_{z \sim_u S} \left[ g(z) \right] = \frac{1}{m} \sum_{i=1}^{m} g(z_i)$$

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Wouldn't it be nice if $\mathop{\mathbb{E}}_{S \sim D^m} \left[ \Phi(S) \right] \leq 2\mathfrak{R}_m(\mathcal{G})$?

# Proof of Main Result

All that remains to show is that $\underset{S \sim D^m}{\mathbb{E}} \left[ \Phi(S) \right] \leq 2\mathfrak{R}_m(\mathcal{G})$

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Introduce a fresh sample $S' \sim D^m$

$$\mathop{\mathbb{E}}_{S\sim D^m}\left[\Phi(S)\right] = \mathop{\mathbb{E}}_{S\sim D^m}\left[\sup_{g\in\mathcal{G}}\left(\mathop{\mathbb{E}}_{S'\sim D^m}\left[\mathop{\widehat{\mathbb{E}}}_{z\sim_u S'}\left[g(z)\right]\right] - \mathop{\widehat{\mathbb{E}}}_{z\sim_u S}\left[g(z)\right]\right)\right]$$

# Proof of Main Result

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Pushing the $\sup$ inside the expectation

$$\mathop{\mathbb{E}}_{S\sim D^m}\left[\Phi(S)\right] \leq \mathop{\mathbb{E}}_{S\sim D^m, S'\sim D^m}\left[\sup_{g\in\mathcal{G}}\left(\mathop{\widehat{\mathbb{E}}}_{z\sim_u S'}\left[g(z)\right] - \mathop{\widehat{\mathbb{E}}}_{z\sim_u S}\left[g(z)\right]\right)\right]$$

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$S$ and $S'$ are identically distributed, so their elements can be swapped by introducing Rademacher random variables $\sigma_i \in \{-1, 1\}$

$$\begin{aligned}\mathop{\mathbb{E}}_{S\sim D^m}\left[\Phi(S)\right] &\leq \mathop{\mathbb{E}}_{S\sim D^m, S'\sim D^m, \boldsymbol{\sigma}}\left[\sup_{g\in\mathcal{G}}\frac{1}{m}\sum_{i=1}^{m}\sigma_i(g(z_i') - g(z_i))\right] \\ &\leq 2\mathop{\mathbb{E}}_{S\sim D^m, \boldsymbol{\sigma}}\left[\sup_{g\in\mathcal{G}}\frac{1}{m}\sum_{i=1}^{m}\sigma_i g(z_i)\right] = 2\mathfrak{R}_m(\mathcal{G})\end{aligned}$$

# Outline

Statistical (Supervised) Learning Theory Framework

Linear Regression

Rademacher Complexity

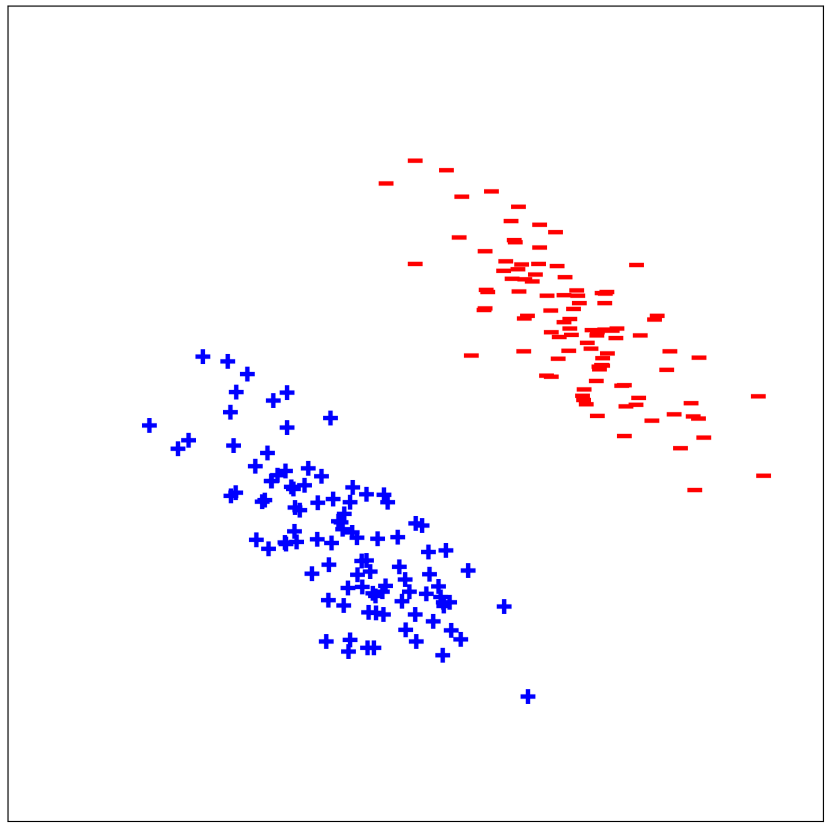
Support Vector Machines

Kernels

Neural Networks

Algorithmic Stability

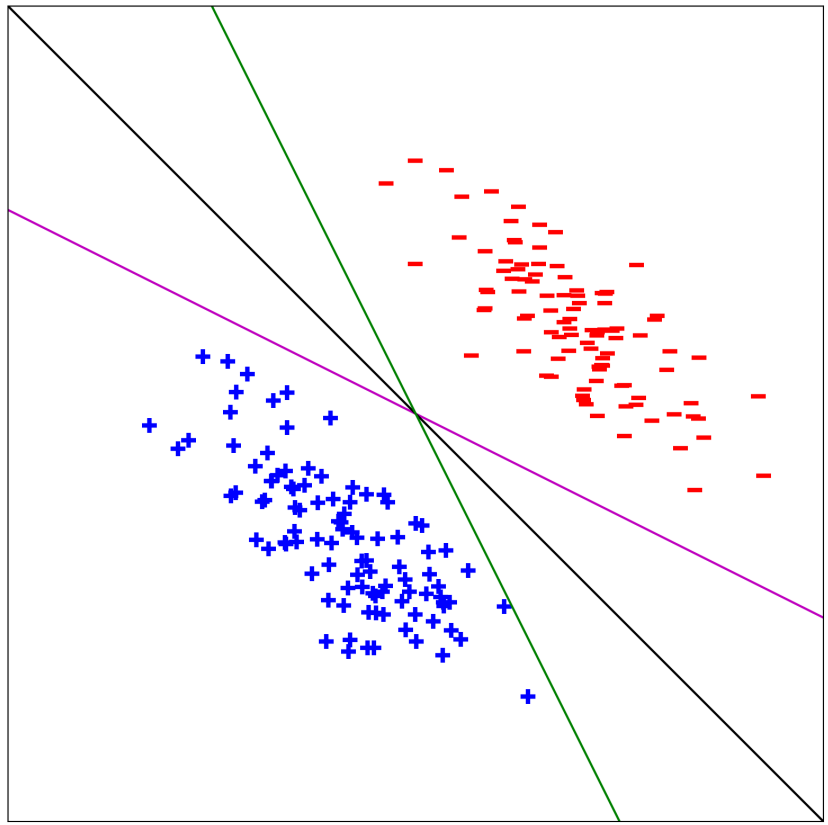
# Support Vector Machines: Binary Classification



Goal: Find a linear separator

Data is linearly separable if there exists a linear separator that classifies all points correctly

# Support Vector Machines: Binary Classification

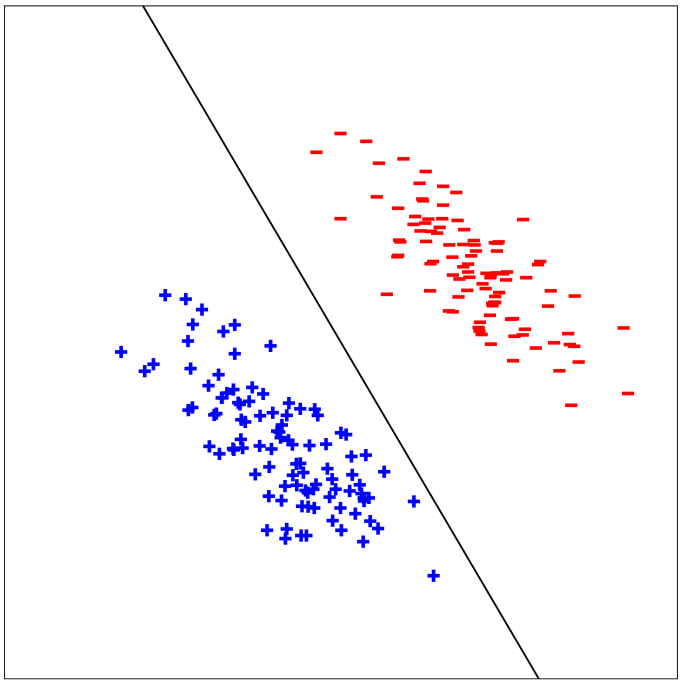


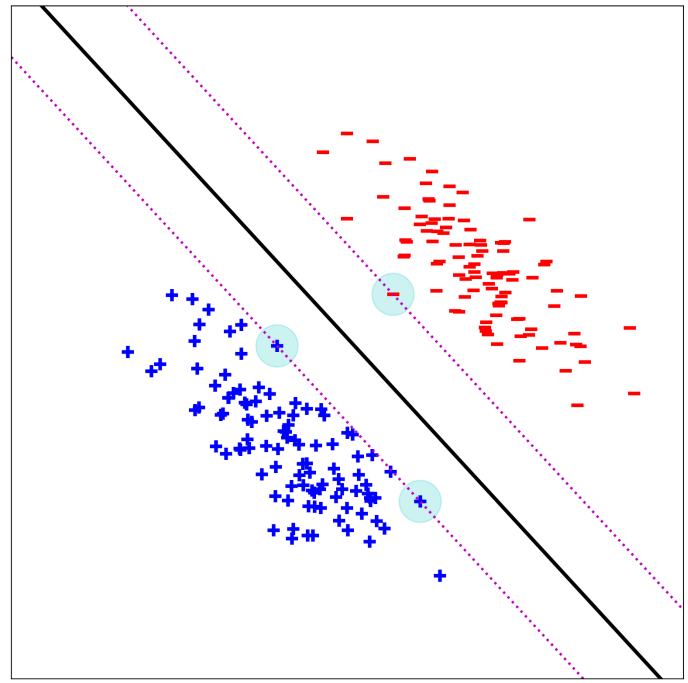
Goal: Find a linear separator

Data is linearly separable if there exists a linear separator that classifies all points correctly

Which separator should be picked?

# Support Vector Machines: Maximum Margin Principle



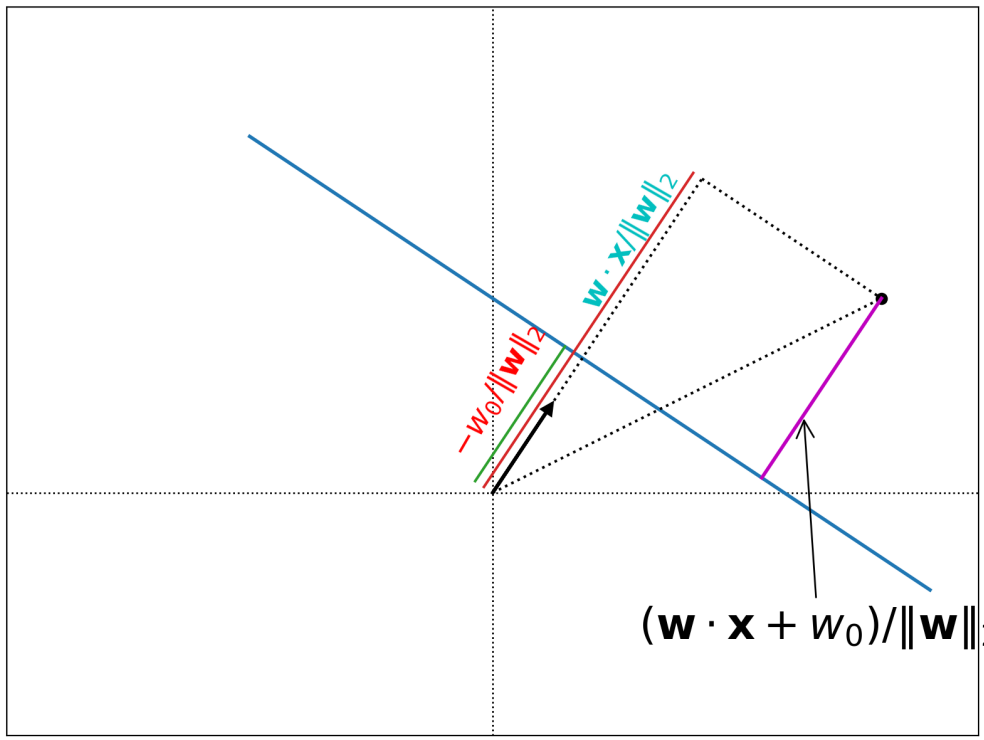


Maximise the distance of the closest point from the decision boundary

Points that are closest to the decision boundary are support vectors

# Support Vector Machines : Geometric View

Given a hyperplane: $H \equiv \mathbf{w} \cdot \mathbf{x} + w_0 = 0$ and a point $\mathbf{x} \in \mathbb{R}^n$, how far is $\mathbf{x}$ from $H$?



# Support Vector Machines : Geometric View

Consider the hyperplane: $H \equiv \mathbf{w} \cdot \mathbf{x} + w_0 = 0$

The distance of point $\mathbf{x}$ from $H$ is given by

$$\frac{|\mathbf{w} \cdot \mathbf{x} + w_0|}{\|\mathbf{w}\|_2}$$

All points on one side of the hyperplane satisfy (labelled $y = +1$)

$$\mathbf{w} \cdot \mathbf{x} + w_0 \geq 0$$

and points on the other side satisfy (labelled $y = -1$)

$$\mathbf{w} \cdot \mathbf{x} + w_0 < 0$$

# SVM Formulation : Separable Case

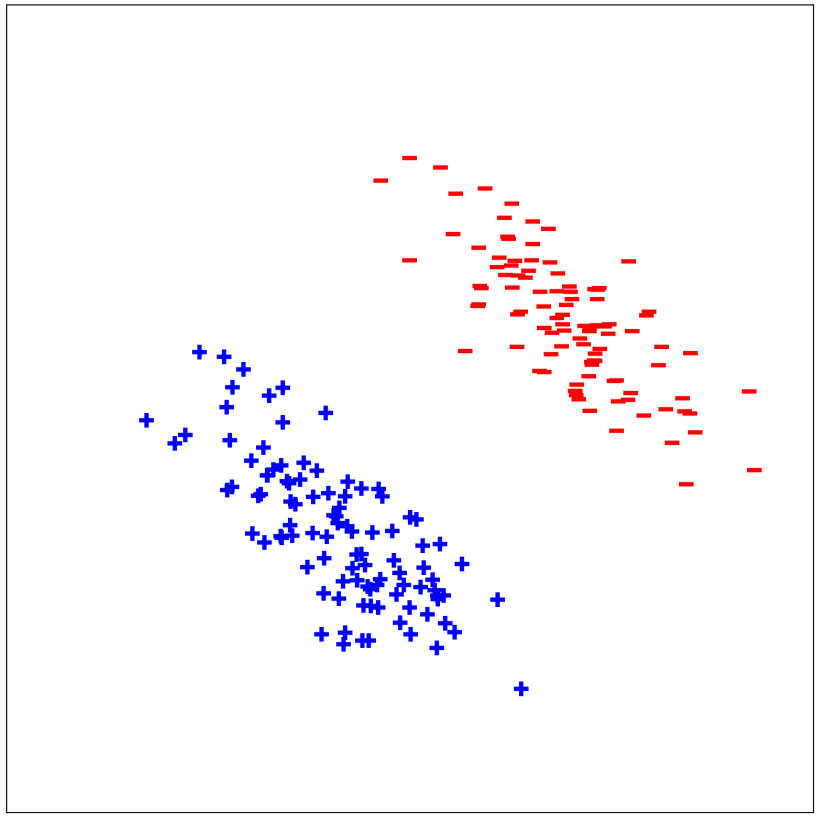
minimise: $\frac{1}{2} \|\mathbf{w}\|_2^2$

subject to:

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) \geq 1$$

for $i = 1, \ldots, m$

Here $y_i \in \{-1, 1\}$



If data is separable, then we find a classifier with no classification error on the training set

The margin of the classifier is $\frac{1}{\|\mathbf{w}^*\|_2}$ if $\mathbf{w}^*$ is the optimal solution

This is a convex quadratic program and hence can be solved efficiently

# SVM Formulation : The Dual

minimise: $\frac{1}{2}\|\mathbf{w}\|_2^2$

subject to:

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) - 1 \geq 0$$

for $i = 1, \ldots, m$

Here $y_i \in \{-1, 1\}$

maximise $$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

subject to:

$$\sum_{i=1}^{m} \alpha_i y_i = 0$$

$$0 \leq \alpha_i$$

for $i = 1, \ldots, m$

## Lagrange Function

$$\Lambda(\mathbf{w}, w_0; \boldsymbol{\alpha}) = \frac{1}{2} \|\mathbf{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i (y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) - 1)$$

## Complementary Slackness

$$\alpha_i (y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) - 1) = 0, \;\; i = 1, \ldots, m$$

# SVM Formulation : Non-Separable Case

minimise: $\frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{m}\zeta_i$

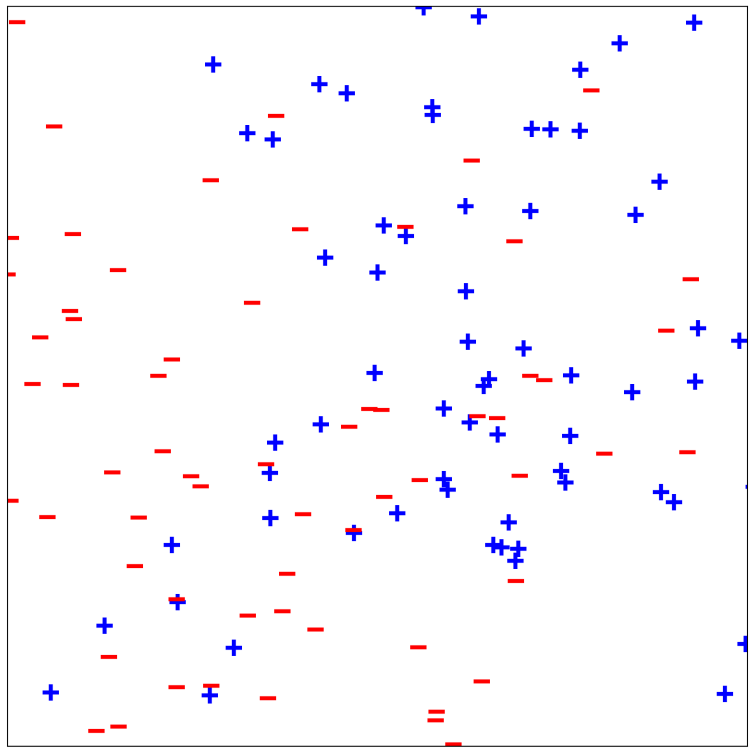
subject to:

$$y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) \geq 1 - \zeta_i$$

$$\zeta_i \geq 0$$

for $i = 1, \ldots, m$

Here $y_i \in \{-1, 1\}$



# SVM Formulation : Loss Function

minimise: $\underbrace{\frac{1}{2}\|\mathbf{w}\|_2^2}_{\text{Regulariser}} + \underbrace{C\sum_{i=1}^{m}\zeta_i}_{\text{Loss Function}}$

subject to:

$$y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) \geq 1 - \zeta_i$$

$$\zeta_i \geq 0$$

for $i = 1, \ldots, m$

Here $y_i \in \{-1, 1\}$

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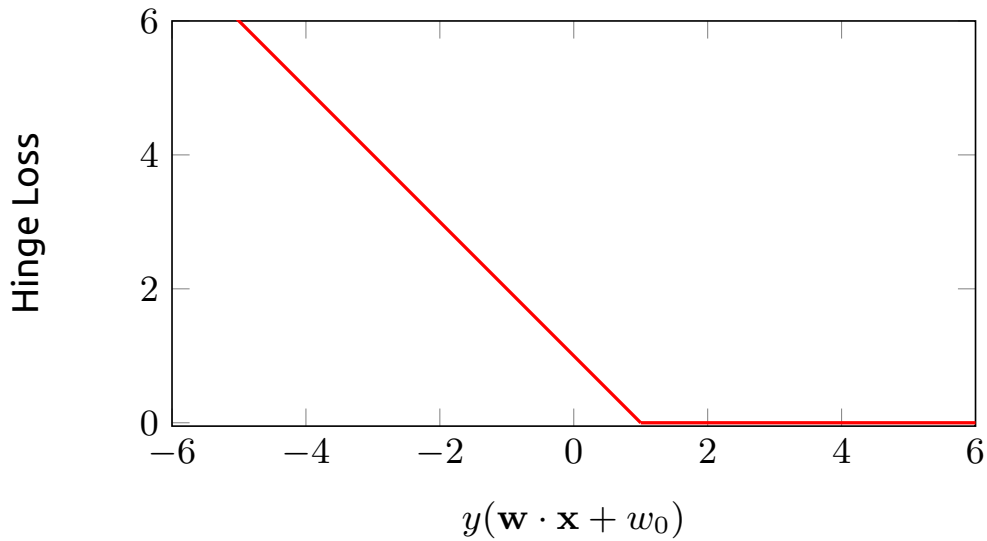

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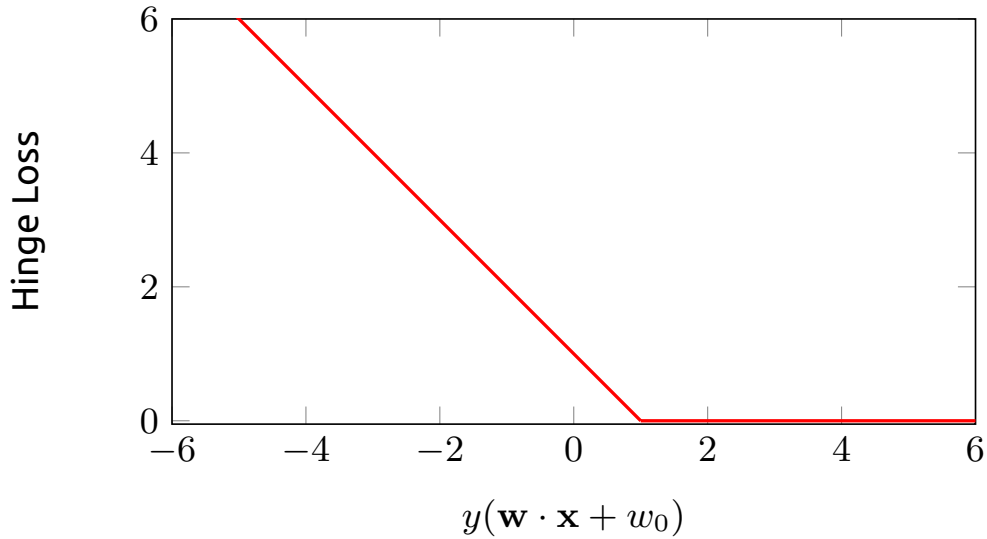


Note that for the optimal solution, $\zeta_i = \max\{0, 1 - y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0)\}$

Thus, SVM can be viewed as minimising the hinge loss with regularisation

# SVM : Deriving the Dual

minimise: $\frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{m}\zeta_i$

subject to:

$y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) - (1-\zeta_i) \geq 0$

$\zeta_i \geq 0$

for $i = 1, \ldots, m$

Here $y_i \in \{-1, 1\}$

## Lagrange Function

$$\Lambda(\mathbf{w}, w_0, \boldsymbol{\zeta}; \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{m}\zeta_i - \sum_{i=1}^{m}\alpha_i(y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) - (1-\zeta_i)) - \sum_{i=1}^{m}\mu_i\zeta_i$$

# SVM : Deriving the Dual

## Lagrange Function

$$\Lambda(\mathbf{w}, w_0, \boldsymbol{\zeta}; \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{m}\zeta_i - \sum_{i=1}^{m}\alpha_i(y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) - (1-\zeta_i)) - \sum_{i=1}^{m}\mu_i\zeta_i$$

We write derivatives with respect to $\mathbf{w}$, $w_0$ and $\zeta_i$,

$$\frac{\partial\Lambda}{\partial w_0} = -\sum_{i=1}^{m}\alpha_i y_i$$

$$\frac{\partial\Lambda}{\partial\zeta_i} = C - \alpha_i - \mu_i$$

$$\nabla_{\mathbf{w}}\Lambda = \mathbf{w} - \sum_{i=1}^{m}\alpha_i y_i \mathbf{x}_i$$

For (KKT) dual feasibility constraints, we require $\alpha_i \geq 0$, $\mu_i \geq 0$

# SVM : Deriving the Dual

Setting the derivatives to $0$, substituting the resulting expressions in $\Lambda$ (and simplifying), we get a function $g(\boldsymbol{\alpha})$ and some constraints

$$g(\boldsymbol{\alpha}) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

## Constraints

$$0 \leq \alpha_i \leq C \qquad\qquad i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0$$

Finding critical points of $\Lambda$ satisfying the KKT conditions corresponds to finding the maximum of $g(\boldsymbol{\alpha})$ subject to the above constraints

# SVM: Primal and Dual Formulations

## Primal Form

minimise: $\frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{m}\zeta_i$

subject to:

$$y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) \geq (1-\zeta_i)$$

$$\zeta_i \geq 0$$

for $i = 1, \ldots, m$

## Dual Form

maximise $\sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_i\alpha_j y_i y_j \mathbf{x}_i\cdot\mathbf{x}_j$

subject to:

$$\sum_{i=1}^{m}\alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C$$

for $i = 1, \ldots, m$

# KKT Complementary Slackness Conditions

For all $i$, $\alpha_i \left( y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) - (1 - \zeta_i) \right) = 0$

If $\alpha_i > 0$, $y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) = 1 - \zeta_i$

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For all $i$, $\alpha_i \left( y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) - (1 - \zeta_i) \right) = 0$

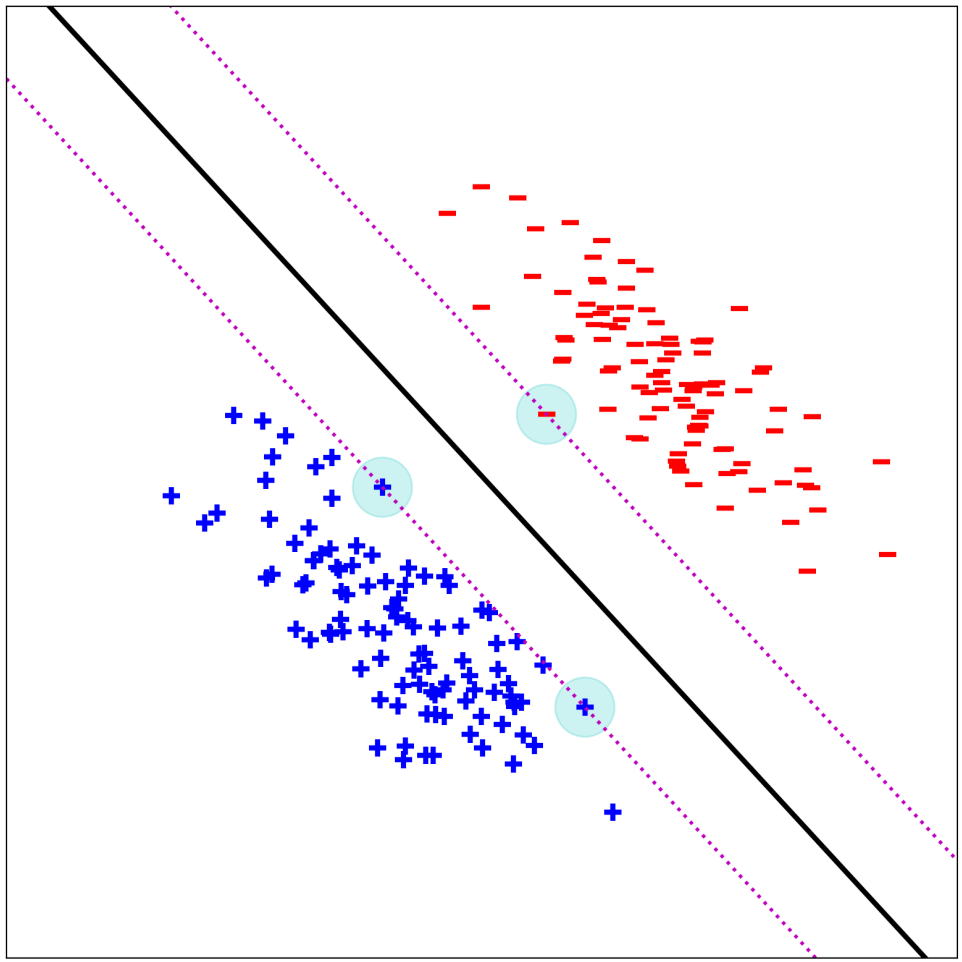
If $\alpha_i > 0$, $y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) = 1 - \zeta_i$

Recall the form of the solution: $\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$

Thus, only those datapoints $\mathbf{x}_i$ for which $\alpha_i > 0$, determine the solution

This is why they are called support vectors

# Support Vectors



# Generalisation Bounds Based on Margin

Suppose we solve the SVM objective by constraining $\mathbf{w}$ to be in the set $\{\mathbf{w} \mid \|\mathbf{w}\|_2 \leq W\}$

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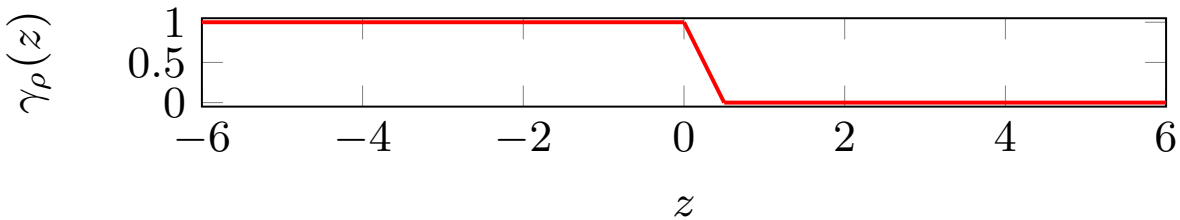
$$\varphi_\rho(z) = \begin{cases} 0 & \text{if } \rho \leq z \\ 1 - z/\rho & \text{if } 0 \leq z \leq \rho \\ 1 & \text{if } z \leq 0 \end{cases}$$



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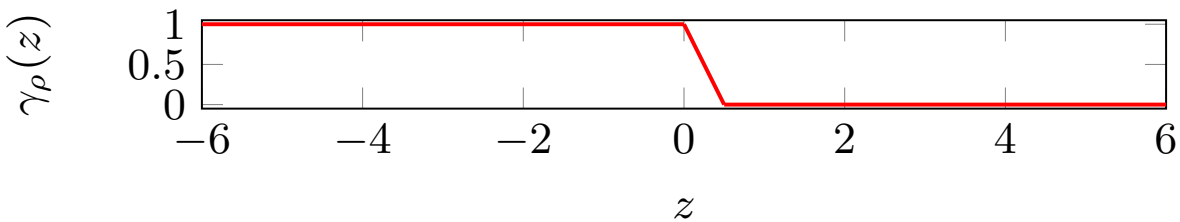


Let $\mathcal{H} = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \mid \|\mathbf{w}\|_2 \leq W\}$ and let $\|\mathbf{x}\|_2 \leq X$ for all $\mathbf{x} \in X$, as $\varphi_\rho$ is $1/\rho$-Lipschitz by Talagrand's Lemma we have

$$\widehat{\mathfrak{R}}(\varphi_\rho \circ \mathcal{H}) \leq \frac{WX}{\rho\sqrt{m}}$$

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Observe that $\gamma(y', y) \leq \gamma_\rho(y', y)$

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Let $R(h_{\mathbf{w}}) = \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim D}\left[\gamma(\text{sign}(\mathbf{w}\cdot\mathbf{x}), y)\right]$ and let
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Then, we have

$$R(h) \leq R_\rho(h) \leq \widehat{R}_\rho(h) + 2\widehat{\mathfrak{R}}(\phi \circ \mathcal{H}) + O\left(\sqrt{\frac{\log(1/\delta)}{m}}\right)$$

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As $\widehat{\mathfrak{R}}(\phi \circ \mathcal{H}) = O(XW/\rho\sqrt{m})$, a sample size of $m = O(W^2X^2/(\rho\epsilon)^2)$ is sufficient to get $\epsilon$ excess risk (over $\widehat{R}_\rho(h)$)

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Let $R(h_{\mathbf{w}}) = \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim D}\left[\gamma(\text{sign}(\mathbf{w}\cdot\mathbf{x}), y)\right]$ and let $R_\rho(h_{\mathbf{w}}) = \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim D}\left[\gamma_\rho(\mathbf{w}\cdot\mathbf{x}, y)\right]$. Let $\widehat{R}$ and $\widehat{R_\rho}$ denote the corresponding empirical risks

Then, we have

$$R(h) \leq R_\rho(h) \leq \widehat{R}_\rho(h) + 2\widehat{\mathfrak{R}}(\phi \circ \mathcal{H}) + O\left(\sqrt{\frac{\log(1/\delta)}{m}}\right)$$

As $\widehat{\mathfrak{R}}(\phi \circ \mathcal{H}) = O(XW/\rho\sqrt{m})$, a sample size of $m = O(W^2X^2/(\rho\epsilon)^2)$ is sufficient to get $\epsilon$ excess risk (over $\widehat{R}_\rho(h)$)

Note that solving the SVM objective is not guaranteed to give $h$ that has the smallest $\widehat{R}(h)$ (the problem of minimising disagreements with a linear separator is NP-hard)

# Outline

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Rademacher Complexity

Support Vector Machines

Kernels

Neural Networks

Algorithmic Stability

# Gram Matrix

If we put the inputs in matrix $\mathbf{X}$, where the $i^{th}$ row of $\mathbf{X}$ is $\mathbf{x}_i^\mathsf{T}$.

$$\mathbf{K} = \mathbf{X}\mathbf{X}^\mathsf{T} = \begin{bmatrix} \mathbf{x}_1^\mathsf{T}\mathbf{x}_1 & \mathbf{x}_1^\mathsf{T}\mathbf{x}_2 & \cdots & \mathbf{x}_1^\mathsf{T}\mathbf{x}_m \\ \mathbf{x}_2^\mathsf{T}\mathbf{x}_1 & \mathbf{x}_2^\mathsf{T}\mathbf{x}_2 & \cdots & \mathbf{x}_2^\mathsf{T}\mathbf{x}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_m^\mathsf{T}\mathbf{x}_1 & \mathbf{x}_m^\mathsf{T}\mathbf{x}_2 & \cdots & \mathbf{x}_m^\mathsf{T}\mathbf{x}_m \end{bmatrix}$$

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We only need the ability to compute inner products to use (dual version of) SVM

# Kernel Trick

Suppose, $\mathbf{x} \in \mathbb{R}^2$ and we perform degree $2$ polynomial expansion, we could use the map:

$$\psi(\mathbf{x}) = \left[1, x_1, x_2, x_1^2, x_2^2, x_1 x_2\right]^\mathsf{T}$$

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If $\mathbf{x} = [x_1, x_2]^\mathsf{T}$ and $\mathbf{x}' = [x_1', x_2']^\mathsf{T}$, then

$$\begin{aligned}\phi(\mathbf{x})^\mathsf{T}\phi(\mathbf{x}') &= 1 + 2x_1x_1' + 2x_2x_2' + x_1^2(x_1')^2 + x_2^2(x_2')^2 + 2x_1x_2x_1'x_2' \\ &= (1 + x_1x_1' + x_2x_2')^2 = (1 + \mathbf{x}\cdot\mathbf{x}')^2\end{aligned}$$

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Instead of spending $\approx n^d$ time to compute inner products after degree $d$ polynomial basis expansion, we only need $O(n)$ time

# Kernel Trick

We can use a symmetric positive semi-definite kernel (Mercer Kernels)

$$\mathbf{K} = \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \kappa(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_1, \mathbf{x}_m) \\ \kappa(\mathbf{x}_2, \mathbf{x}_1) & \kappa(\mathbf{x}_2, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_2, \mathbf{x}_m) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(\mathbf{x}_m, \mathbf{x}_1) & \kappa(\mathbf{x}_m, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_m, \mathbf{x}_m) \end{bmatrix}$$

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The dual program becomes

maximise $\sum_{i=1}^{m} \alpha_i - \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j K_{i,j}$

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To make prediction on new $\mathbf{x}_{\text{new}}$, only need to compute $\kappa(\mathbf{x}_i, \mathbf{x}_{\text{new}})$ for support vectors $\mathbf{x}_i$ (for which $\alpha_i > 0$)

# Polynomial Kernels

Rather than perform basis expansion,

$$\kappa(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x} \cdot \mathbf{x}')^d$$

This gives all terms of degree up to $d$

If we use $\kappa(\mathbf{x}, \mathbf{x}') = (\mathbf{x} \cdot \mathbf{x}')^d$, we get only degree $d$ terms

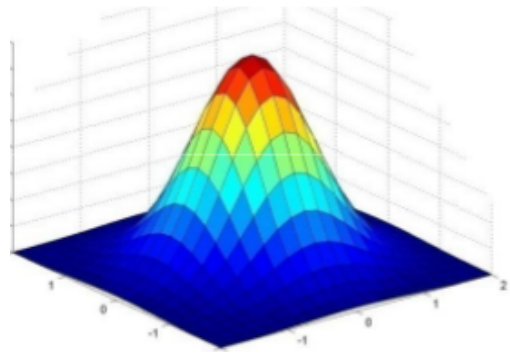
Linear Kernel: $\kappa(\mathbf{x}, \mathbf{x}') = \mathbf{x} \cdot \mathbf{x}'$

All of these satisfy the Mercer or positive-definite condition

# Gaussian or RBF Kernel

Radial Basis Function (RBF) or Gaussian Kernel

$$\kappa(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right)$$



$\sigma^2$ is known as the bandwidth

Can generalise to more general covariance matrices

Results in a Mercel kernel

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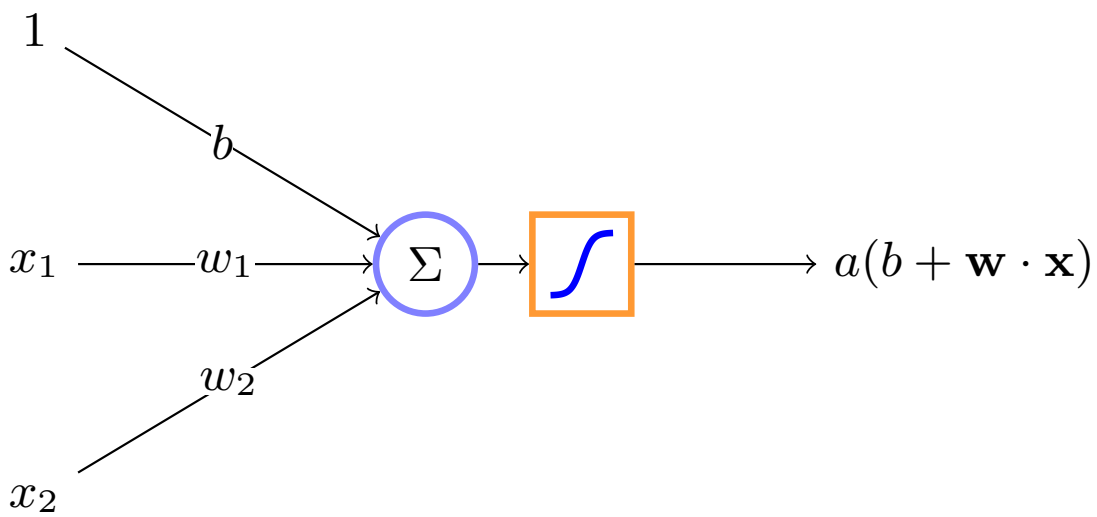
# Neural Networks : Unit



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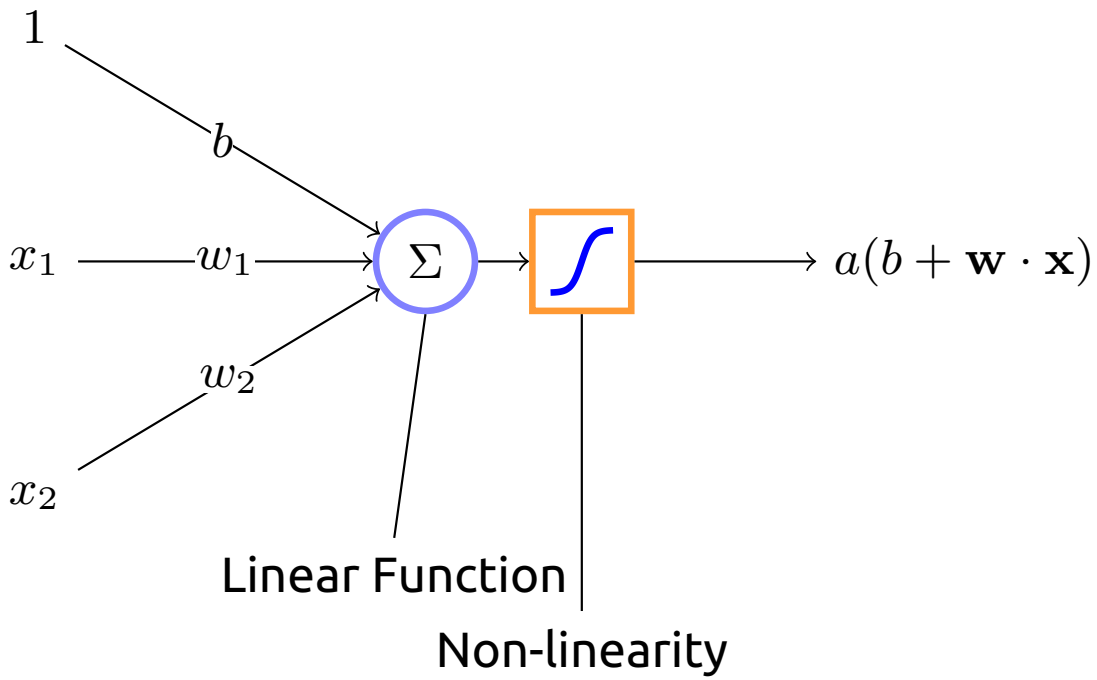

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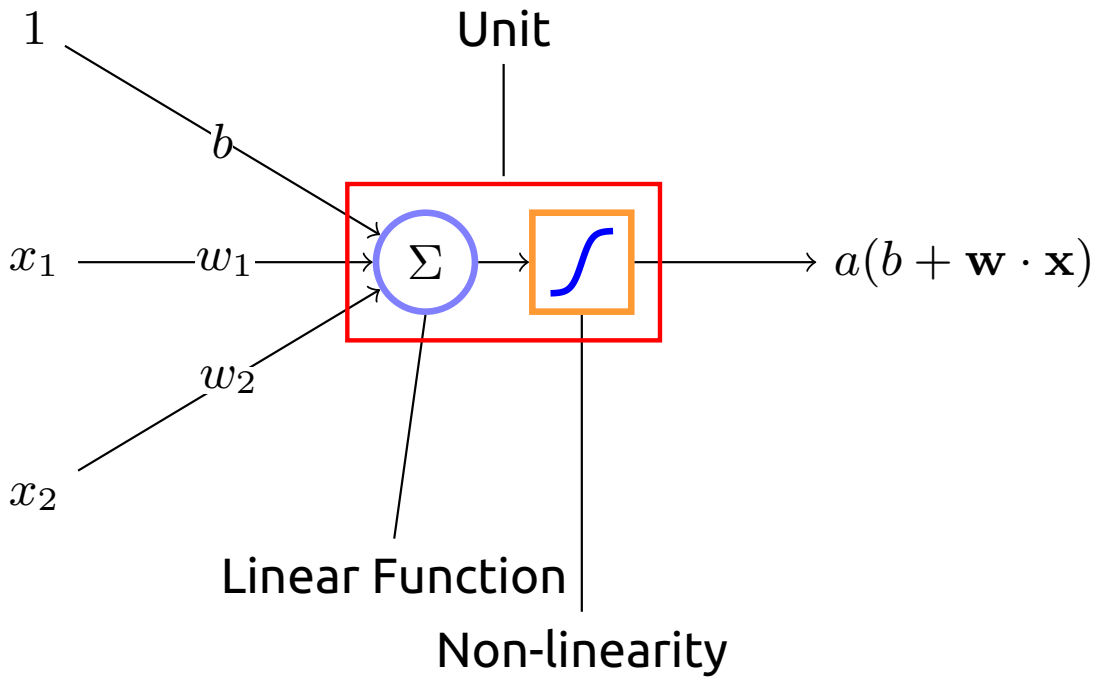

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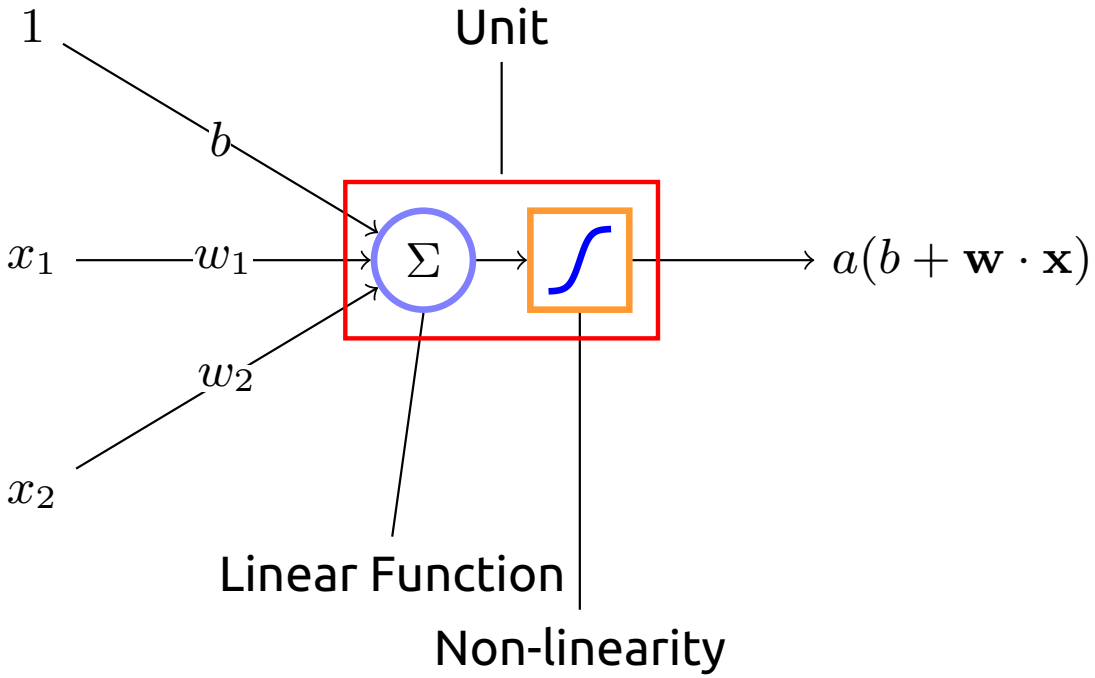
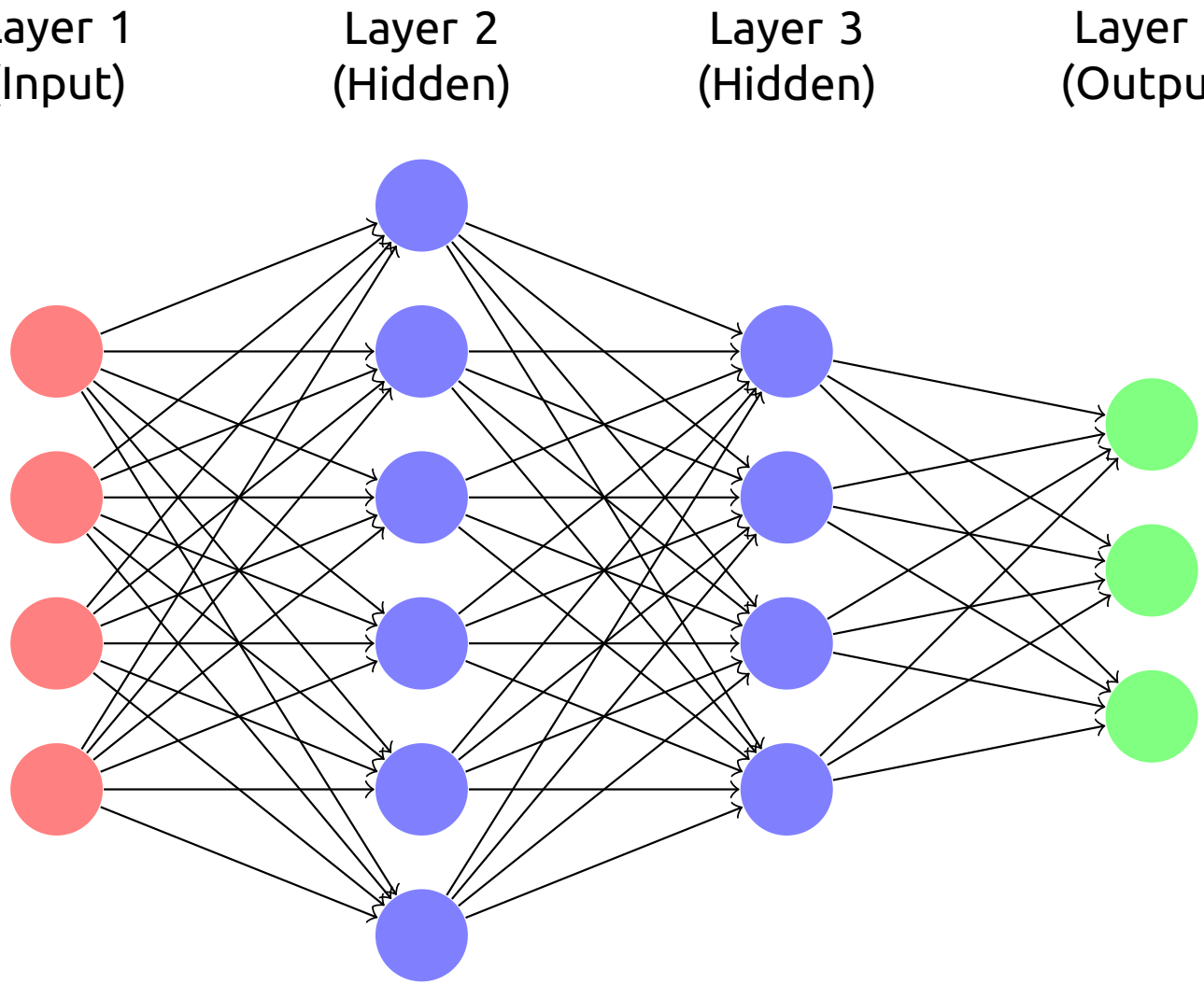



A unit in a neural network computes an affine function of its input and is then composed with a non-linear activation function $a$

For example the activation function could be the logistic sigmoid

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

# Feedforward Neural Networks



# Neural Networks

Only consider fully-connected, feed-forward neural networks, with non-linear activation functions applied element-wise to units

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A layer $l : \mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$ consists of an element-wise composition of a non-linear activation $a$, e.g. rectifier or logistic sigmoid, and an affine map

$$l(\mathbf{z}) = a(W\mathbf{z} + \mathbf{b})$$

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An $L$-hidden layer network represents a function $f : \mathbb{R}^n \to \mathbb{R}$

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Typically, the output layer is simply an affine map of the penultimate layer (without any non-linear activation)

# Capacity of Neural Networks

**VC dim. of Neural Nets**

Informally, if $a$ is the $\mathrm{sgn}$ function, and $C$ is the class of all neural networks with at most $\omega$ parameters then, $\mathrm{VC}(C) \leq 2\omega \log_2(e\omega)$

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## Rademacher Complexity of Neural Nets

Suppose $\mathcal{F}$ is the class of feed-forward neural nets with $L-1$ hidden layers

- every row of $\mathbf{w}$ of any $W$ in the net satisfying $\|\mathbf{w}\|_1 \leq W$

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Then, $\widehat{\mathfrak{R}}_m(\mathcal{F}) \leq \frac{1}{\sqrt{m}} \left( (2W)^L + B \sum_{i=0}^{L-1} (2W)^i \right)$

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Exercise: Prove this using the fact that if $\overline{\mathcal{G}}$ is the function class consisting of all convex combinations of functions in $\mathcal{G}$, then $\widehat{\mathfrak{R}}_m(\overline{\mathcal{G}}) = \widehat{\mathfrak{R}}(\mathcal{G})$. (Also prove the latter claim.)

# Neural Networks : Universality Results

**(Simplified) Theorem (Cybenko)** [6]

Let $\sigma$ be the logistic sigmoid activation function. Then the set of functions of the form $G(\mathbf{x}) = \sum_{i=1}^{N} \alpha_j \sigma(\mathbf{w}_j \cdot \mathbf{x} + b_j)$ are dense in the set of continuous functions on $[0, 1]^n$.

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These kinds of results don't inform us directly about the success of training algorithms or the possibility of generalisation

# Depth Separation Results

Universality results establish that neural nets with one hidden layer are universal approximators

Establishing the benefits of depth (both for representation and learning) is an active area of research

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Eldan and Shamir[7] established the existence of a function that can be well approximated by a depth-3 (2 hidden layers) neural network using polynomially many units (in dimension), but requires exponentially many units using a depth-2 network

Telgarsky[15] established for each $k \in \mathbb{N}$, the existence of a function that can be well approximated by a depth-$k^3$ neural network using polynomially many units (in dimension and $k$), but requires exponentially many units using a depth-$k$ neural network

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So far we have seen uniform convergence bounds, i.e. bounds of the form that "under suitable conditions" with high probability, $\forall f \in \mathcal{F}$,

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Q. Can analysing learning algorithms directly yield a (possibly different/better) way to obtain bounds on the true risk?

# Algorithmic Stability

Let $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ be a sample drawn from $D$ over $\mathcal{X} \times \mathcal{Y}$ and $S'$ be a sample that differs from $S$ on exactly one point, say it has $(\mathbf{x}'_m, y'_m)$ instead of $(\mathbf{x}_m, y_m)$

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A learning algorithm $A$ is uniformly $\beta$-stable if for any samples $S, S'$ of size $m$, differing in exactly one point, it holds for every $(\mathbf{x}, y)$ that:

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**Theorem (Bousquet & Elisseeff)** [3]

Suppose $\gamma$ is a bounded cost function $|\gamma| \leq M$ and that $A$ is uniformly $\beta$-stable. Let $S \sim D^m$, then for every $\delta > 0$, with probability at least $1 - \delta$, it holds that:

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Cannot be used for zero-one classification loss

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The ridge regression method finds

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**Theorem.** Since $\gamma$ is convex and $\sigma$-admissible, ridge regression is uniformly $\beta$-stable with $\beta \leq \frac{\sigma^2 X^2}{m\lambda} = O(1/m)$

Recent work by Hardt et al.[9] has shown that stochastic gradient descent (with early stopping) is uniformly stable

# Summary

Uniform convergence bounds for bounding generalisation error using Rademacher complexity bounds

Application of Rademacher complexity bounds to Linear Regression, GLMs, SVMs

A brief view of some results about neural networks

Algorithmic stability as a means to bound generalisation error

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