Learning in Big Data Analytics
Lecture 2

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Supervised Learning

Supervised Learning

- There is a functional relationship

$$f^* : \mathbb{R}^d \to V$$

we would like to understand, or *learn*.
  - *Regression*: $V = \mathbb{R}$
  - *Classification*: $V = \{1, ..., k\}$
- To learn it, we are given *m data points*

$$(x_i, f^*(x_i) = y_i)_{i=1,...,m}$$

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that reflect this functional relationship.

Final goal: Predict $f^*(x)$ well on unknown data points x.

Supervised versus Unsupervised Learning

- *Unsupervised Learning:*
  - Given unlabeled data

$$(x_i)_{i=1,\ldots,m}$$

  - *Goal:* Infer subgroups of data points
  - *Alternative Problem Formulation:* Learn the probability distribution

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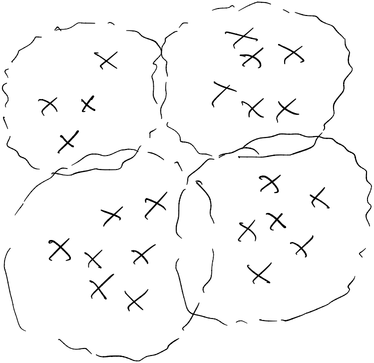

Supervised versus Unsupervised Learning

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  - Given labeled data
    $$(x_i, y_i)_{i=1,\dots,m}$$
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  - *Alternative Problem Formulation:* Learn the probability distribution
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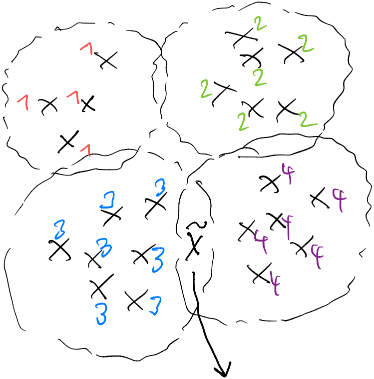

$$P(3 \mid \tilde{x}) \approx 0.5$$

$$P(4 \mid \tilde{x}) = 0.5$$

SUPERVISED LEARNING: TRAINING

- The idea is to set up a *training procedure* (an algorithm) that *learns* f^* from the training data.
- Learning f^* means to *approximate* it by $f : \mathbb{R}^d \to V$ sufficiently well, where $f \in \mathcal{M}$ for a certain class of functions $\mathcal{M}$.
- In most cases, $f \in \mathcal{M}$ are parameterized by parameters $\mathbf{w}$. This means that we have to pick an appropriate choice of parameters $\mathbf{w}$ for learning f^*.

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Supervised Learning

- We need to determine a *cost (or loss) function* C where $C(f, f^*)$ measures how well $f \in \mathcal{M}$ approximates f^*.
- *Optimization*: Pick $f \in \mathcal{M}$ (by picking the right set of parameters) that yields small (possibly minimal) cost $C(f, f^*)$
- *Generalization*: Optimization procedure should address that f is to approximate f^* well on *unknown data points*.

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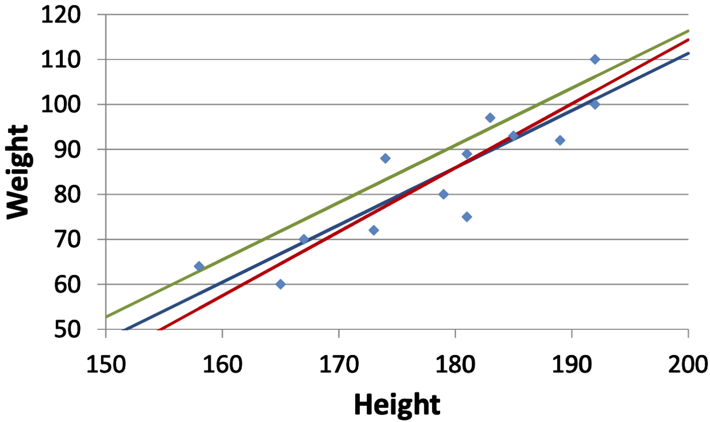
Linear Regression

Example: $f : \mathbb{R} \rightarrow \mathbb{R}$



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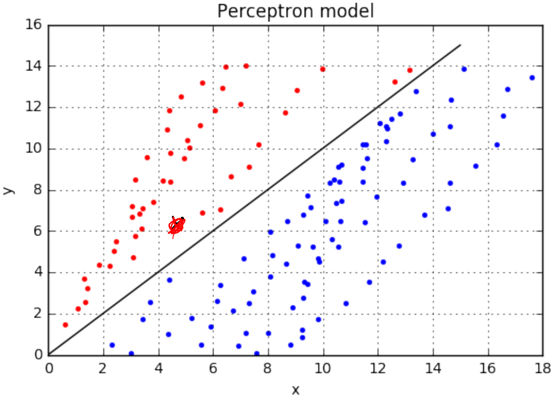
EXAMPLE: $f : \mathbb{R}^2 \to \{0, 1\}$



$$\begin{aligned} f \quad & \mathbb{R}^2 && \longrightarrow && \{0 = \text{blue}, 1 = \text{red}\} \\ & (x_1, x_2) && \mapsto && \begin{cases} 1 & x_2 - x_1 > 0 \\ 0 & x_2 - x_1 \leq 0 \end{cases} \end{aligned} \tag{1}$$

We need to specify:

- How to set up the data being used for training
- A model class $\mathcal{M}$, for example linear functions
- A cost function $C(f, f^*)$ that evaluates the goodness of $f \in \mathcal{M}$
- An optimization procedure that picks f such that $C(f, f^*)$ is minimal, or very small
- Keep in mind that f is to perform well on previously unseen data

Supervised Learning

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- The dataset is given by a *design matrix* $\mathbf{X} \in \mathbb{R}^{m \times d}$ where m is the number of data points and d is the number of *features*
- Each data point x_i (a row in $\mathbf{X}$) is assigned to a *label* y_i that reflects the true functional relationship $y_i = f^*(x_i)$, where further $\mathbf{y} = (y_1, ..., y_m) \in V^m$ is the *label vector*.

Supervised Learning

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Generalization

Enabling Generalization: Data

Training, Test and Validation

- Split $(\mathbf{X}, \mathbf{y})$ into
  - training data $(\mathbf{X}^{(\text{train})}, \mathbf{y}^{(\text{train})})$
  - validation data $(\mathbf{X}^{(\text{val})}, \mathbf{y}^{(\text{val})})$
  - test data $(\mathbf{X}^{(\text{test})}, \mathbf{y}^{(\text{test})})$
- While *training data* is to pick the optimal set of parameters (which specify elements from $\mathcal{M}$), using training and *validation data* in combination is for picking *hyperparameters*
- Hyperparameters can refer to choosing subsets of $\mathcal{M}$. For example, depth of a neural network, and widths of hidden layers. They may also refer to specifications of cost function or optimization procedure.
- $(\mathbf{X}^{(\text{test})}, \mathbf{y}^{(\text{test})})$ are never touched during training.
- The final goal is to minimize the cost on the test data.

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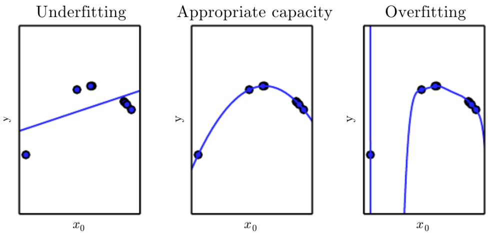
Enabling Generalization: Model

Capacity, Under- and Overfitting



Left: Linear functions underfit
Center: Polynomials of degree 2 neither under- nor overfit
Right: Polynomials of degree 9 overfit

- Choose a class of models that has the right *capacity*
- Capacity too large: *overfitting*
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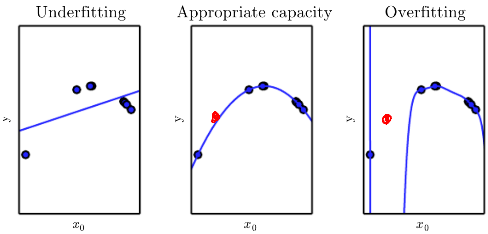

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Enabling Generalization: Cost Function

Regularization

Let $C(f, f^*)$ be the cost function. Let $\mathbf{w} = (w_1, ..., w_k)$ be the parameters specifying elements of $f_\mathbf{w} \in \mathcal{M}$.

- Usually, C refers to only known data points. That is, C evaluates as

$$C(f, f^*) = \sum_i C(f(x_i), y_i = f^*(x_i)) \quad (2)$$

where x_i runs over all training data points.

- Add a *regularization term* to cost function, and choose $f_\mathbf{w}$ that yields minimal

$$C(f_\mathbf{w}, f^*) + \lambda\Omega(\mathbf{w}) \quad (3)$$

- λ is a hyperparameter

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- Prominent examples:
  - *L_1 norm*: $\Omega(\mathbf{w}) := \sum_i |w_i|$
  - *L_2 norm*: $\Omega(\mathbf{w}) := \sum_i w_i^2$
- Rationale: Penalize too many non-zero weights
- Virtually less complex model, hence virtually less capacity
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Enabling Generalization: Optimization

Early Stopping, Dropout

Optimization can be an iterative procedure.

- *Early stopping*: Stop the optimization procedure before cost function reaches an optimum on the training data.
- *Dropout*: Randomly fix parameters to zero, and optimize remaining parameters.

Prominent Supervised Learning Model Examples

Linear Regression

- Design matrix $\mathbf{X} \in \mathbb{R}^{m \times d}$, label vector $\mathbf{y} \in \mathbb{R}^m$
- Model class: Let $\mathbf{w} \in \mathbb{R}^d$

$$f_{\mathbf{w}} = f(\mathbf{x}; \mathbf{w}) : \begin{array}{ccc} \mathbb{R}^d & \longrightarrow & \mathbb{R} \\ \mathbf{x} & \mapsto & \mathbf{w}^T \mathbf{x} \end{array} = \sum_{j=1}^{d} w_j x_j \tag{4}$$

- *Remark*: Note that the case $\mathbf{w}^T\mathbf{x} + b$ can be treated as a special case to be included in $\mathcal{M}$, by augmenting vectors $\mathbf{x}_i$ by an entry 1 (think about this...)
- Cost function (recall $y_i = f^*(\mathbf{x}_i)$)

$$C(f, f^*) := \frac{1}{m} ||(f(\mathbf{x}_1), ..., f(\mathbf{x}_m)) - \mathbf{y}||_2^2 = \frac{1}{m} \sum_{i=1}^{m} (f(\mathbf{x}_i) - \mathbf{y}_i)^2 \tag{5}$$

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Linear Regression

Optimization

- Solve for

$$\nabla_{\mathbf{w}} C(f_{\mathbf{w}}, f^*) = 0 \tag{6}$$

  to achieve a minimum. This yields the *normal equations*

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \tag{7}$$

- *Global optimum* if $\mathbf{X}^T\mathbf{X}$ is invertible
- Do this on *training data* (so $\mathbf{X} = \mathbf{X}^{(\text{train})}, \mathbf{y} = \mathbf{y}^{(\text{train})}$) only. Hope that cost on test data is small.

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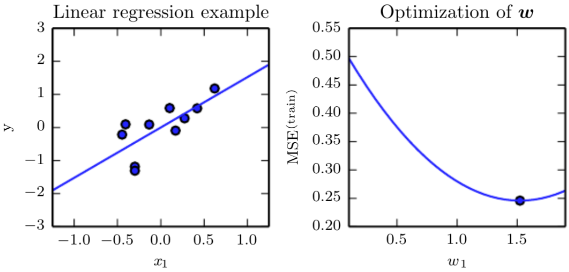
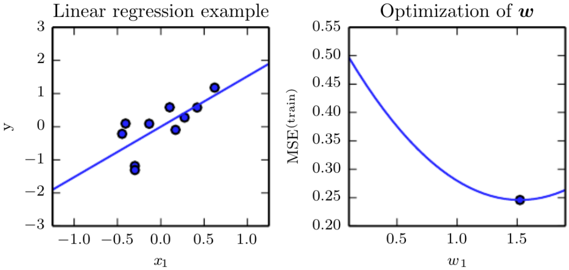


- *Left*: Data points, and the linear function $y = w_1 x$ that approximates them best
- *Right*: Mean squared error (MSE) depending on w_1
- *Remark on Perceptrons*: Optimizing is different, but also supported by a very easy optimization scheme (the *perceptron algorithm*)

NORMAL EQUATIONS



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Nearest Neighbor Classification

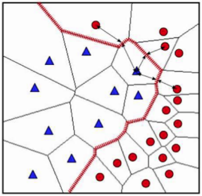
- Consider appropriate distance measure

$$D : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}_+ \quad (8)$$

- For unknown data point $\mathbf{x}$, determine the closest given data point

$$\mathbf{x}_{i^*} := \mathrm{argmin}_i(D(\mathbf{x}, \mathbf{x}_i)) \quad (9)$$

- Predict label of $\mathbf{x}$ as y_{i^*}



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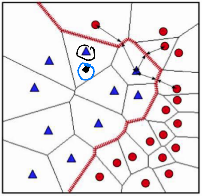


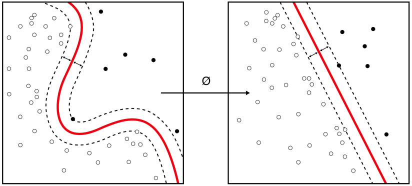
Support Vector Machines

- *Realization*: From (7), write

$$\mathbf{w}^T\mathbf{x} = \sum_{i=1}^{m} \alpha_i \mathbf{x}^T \mathbf{x}_i = \sum_{i=1}^{m} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle \tag{10}$$

- Replace $\langle ., . \rangle$ by different *kernel* (i.e. scalar product) $k(., .)$, that is by computing $\langle \phi(.), \phi(.) \rangle$ for appropriate ϕ

☞ Seek α's to maximize margin: still easy to optimize both for regression and classification!



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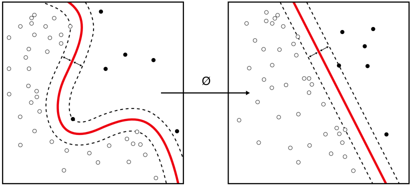


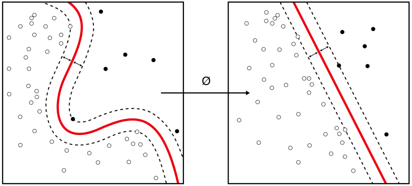
Support Vector Machines

- *Realization*: From (7), write

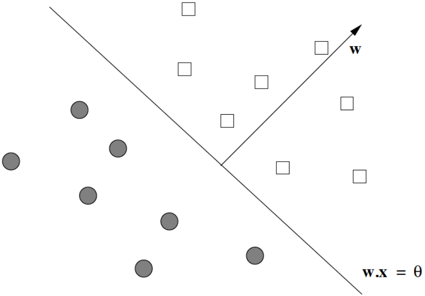
$$\mathbf{w}^T\mathbf{x} = \sum_{i=1}^{m} \alpha_i \mathbf{x}^T \mathbf{x}_i = \sum_{i=1}^{m} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle \qquad (10)$$

- Replace $\langle ., . \rangle$ by different *kernel* (i.e. scalar product) $k(., .)$, that is by computing $\langle \phi(.), \phi(.) \rangle$ for appropriate ϕ

☞ Seek α's to maximize margin: still easy to optimize both for regression and classification!

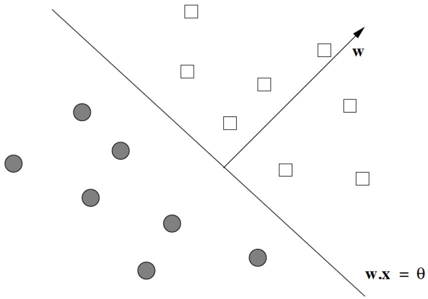


Perceptron Revisited



- A perceptron divides the space into two half spaces
- Half spaces capture the two different classes
- Normal vector alternative description of half space

PERCEPTRON REVISITED



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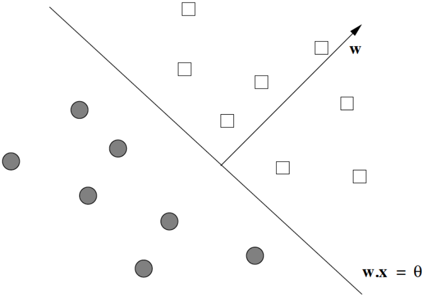

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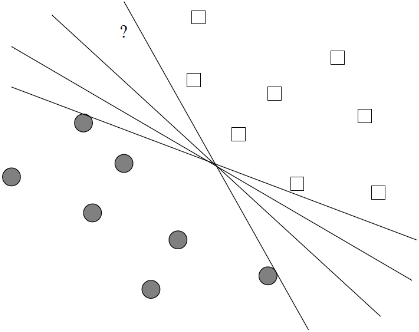

- Several half spaces (normal vectors) divide training data
- *Question:* any half space optimal, in a sensibly defined way?
- What to do if data cannot be separated (is *non-separable*)?

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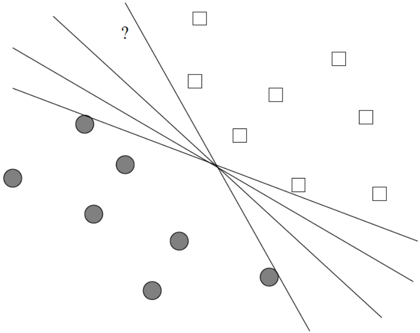

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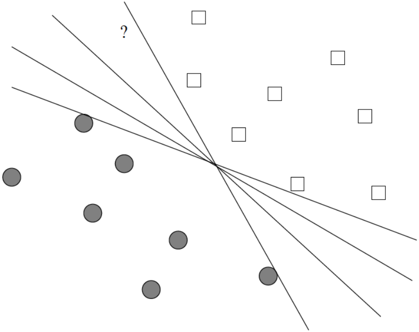

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Support Vector Machines: Motivation

- Support vector machines (SVM's) address to choose most reasonable half space
- SVM's choose half space that maximizes the *margin*
- If separable, maximize distance between hyperplane and closest data points
- If not separable, minimize *loss function* that
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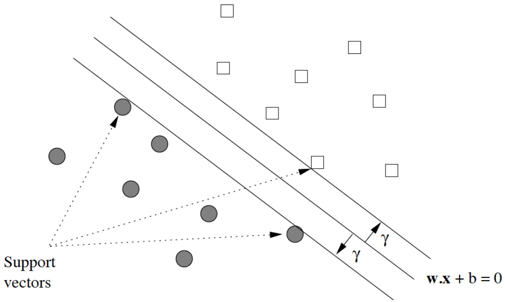
Separable Data



- *Goal:* Select hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 0$ that maximizes distance γ
- *Intuition:* The further away data from hyperplane, the more certain their classification
- Increases chances to correctly classify unseen data (to generalize)

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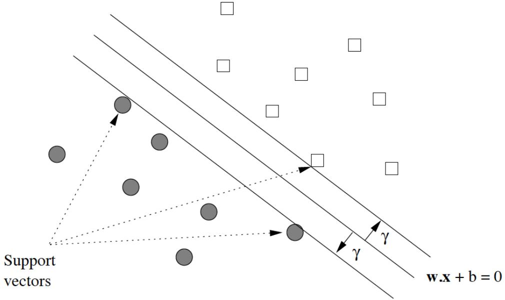

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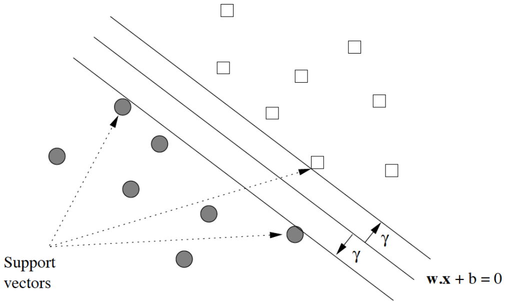
Support Vectors



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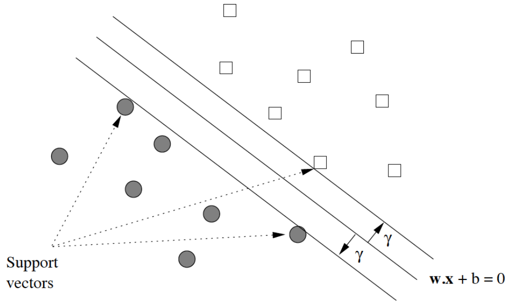

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PROBLEM FORMULATION: FIRST TRY

Let $(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)$ be a training data set, where $\mathbf{x}_i \in \mathbb{R}^d, y_i \in \{-1, +1\}, i = 1, ..., n$.

PROBLEM: By varying $\mathbf{w}, b$, maximize γ such that

$$y_i(\mathbf{w}\mathbf{x}_i + b) \geq \gamma \quad \text{for all } i = 1, ..., n \tag{11}$$

Problem Formulation: First Try

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Problem badly formulated ☞ try harder!

Problem Formulation: Solution

- Data set $(\mathbf{x}_i, y_i), i = 1, ..., n$ as before
- *Solution:* Impose additional constraint: consider only combinations $\mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$ such that for support vectors $\mathbf{x}$

$$y_i(\mathbf{w}\mathbf{x} + b) \in \{-1, +1\} \quad (12)$$

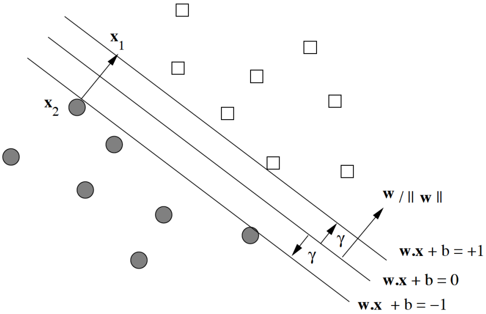
- *Good Formulation:* By varying $\mathbf{w}, b$, maximize γ such that

$$d(x_i, H) \geq \gamma \quad ~~y_i(\mathbf{w}\mathbf{x}_i + b) \geq \gamma~~ \quad \text{for all } i = 1, ..., n \quad (13)$$

and (12) applies

where $d(x_i, H) := \min_x \{ d(x_i, x) \mid wx + b = 0 \}$ is the distance of x_i to the hyperplane $H := \{ x \mid wx + b = 0 \}$

Alternative Problem Formulation I



- $\mathbf{w}, b, \gamma$ determined according to (12),(13)
- $\mathbf{x}_2$ is support vector on lower hyperplane, so by (12), $\mathbf{w}\mathbf{x}_2 + b = -1$
- Let $\mathbf{x}_1$ be the projection of $\mathbf{x}_2$ onto upper hyperplane:

$$\mathbf{x}_1 = \mathbf{x}_2 + 2\gamma \frac{\mathbf{w}}{||\mathbf{w}||} \quad (14)$$

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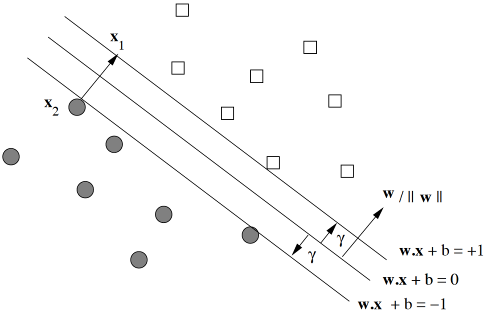

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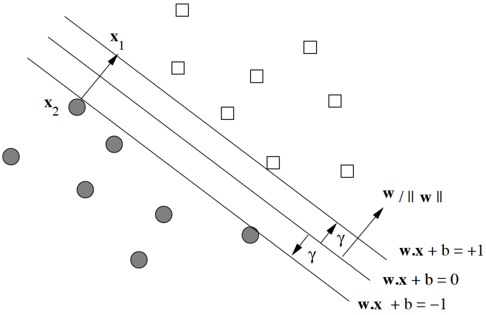
ALTERNATIVE PROBLEM FORMULATION I



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Alternative Problem Formulation II

That is, further, $\mathbf{x}_1$ is on the hyperplane defined by $\mathbf{w}\mathbf{x} + b = 1$, meaning

$$\mathbf{w}\mathbf{x}_1 + b = 1 \tag{15}$$

Alternative Problem Formulation II

That is, further, $\mathbf{x}_1$ is on the hyperplane defined by $\mathbf{wx} + b = 1$, meaning

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Substituting (14) into (15) yields

$$\mathbf{w} \cdot (\mathbf{x}_2 + 2\gamma \frac{\mathbf{w}}{||\mathbf{w}||}) + b = 1 \tag{16}$$

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Because $\mathbf{ww} = ||\mathbf{w}||^2$, by further regrouping, we conclude that

$$\gamma = \frac{1}{||\mathbf{w}||} \tag{18}$$

Alternative Problem Formulation III

Let dataset $(\mathbf{x}_i, y_i), i = 1, ..., n$ be as before.

Equivalent Problem Formulation:

By varying $\mathbf{w}, b$, minimize $||\mathbf{w}||$ subject to

$$y_i(\mathbf{w}\mathbf{x}_i + b) \geq 1 \quad \text{for all } i = 1, ..., n \tag{19}$$

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Optimizing under Constraints

- Topic is broadly covered
- Many packages can be used
- Target function $\sum_i w_i^2$ quadratic; well manageable

Example

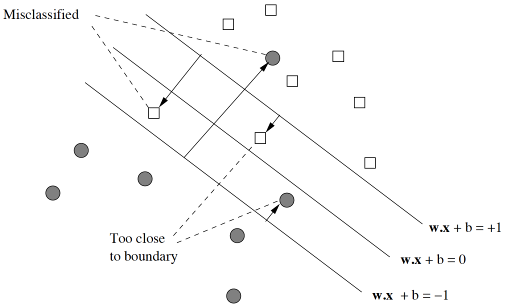
See Example 12.8

in mnds.org

↓

see link in last slide

NON SEPARABLE DATA SETS



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  ☞ *bad points*
- *Non separable data:* any choice of **w**, *b* yields bad points

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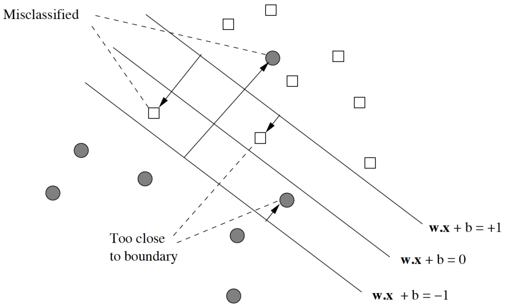

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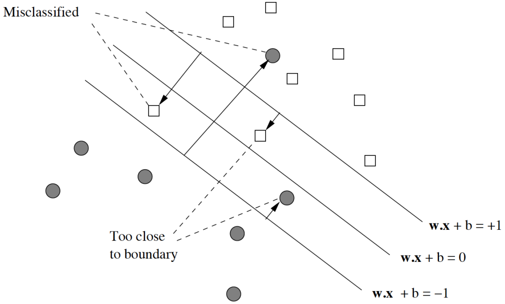

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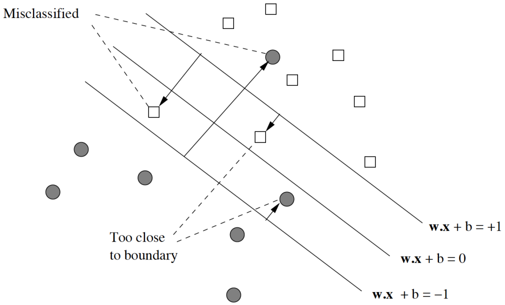

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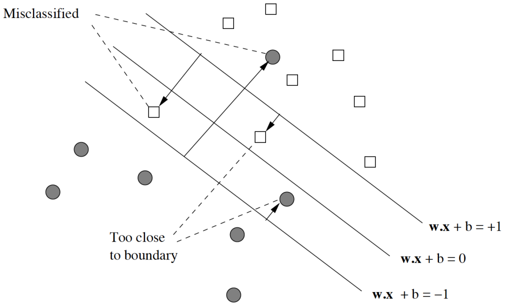

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Let $(\mathbf{x}_i, y_i), i = 1, ...n$ be training data, where

- $\mathbf{x}_i = (x_{i1}, ..., x_{id})$,
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and let $\mathbf{w} = (w_1, ..., w_d)$.

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Minimize the following function:

$$f(\mathbf{w}, b) = \frac{1}{2}\sum_{j=1}^{d} w_j^2 + C\sum_{i=1}^{n} \max\{0, 1 - y_i(\sum_{j=1}^{d} w_j x_{ij} + b)\} \tag{20}$$

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- Minimizing $||\mathbf{w}||$ equivalent to minimizing monotone function of $||\mathbf{w}||$
  ☞ Minimizing f seeks minimal $||\mathbf{w}||$
- Vectors $\mathbf{w}$ and training data balanced in terms of basic units:

$$\frac{\partial(||\mathbf{w}||^2/2)}{\partial w_i} = w_i \quad \text{and} \quad \frac{\partial(\sum_{j=1}^{d} w_j x_{ij} + b)}{\partial w_i} = x_{ij}$$

- C is a regularization parameter
  - Large C: minimize misclassified points, but accept narrow margin
  - Small C: accept misclassified points, but widen margin

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Let the *hinge function* L be defined by

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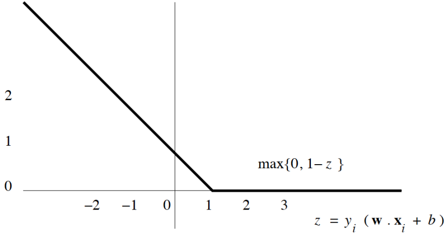

- $L(\mathbf{x}_i, y_i) = 0$ iff $\mathbf{x}_i$ on the correct side of hyperplane with sufficient margin
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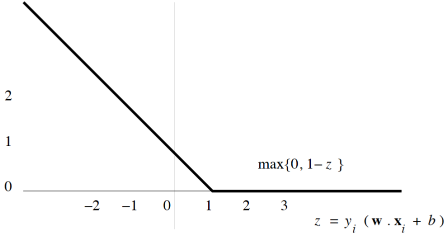

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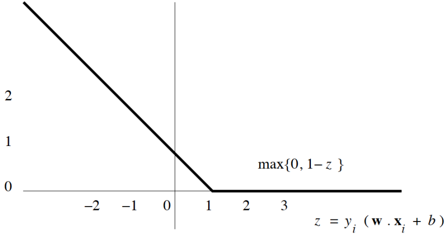

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Partial derivatives of hinge function:

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Reflecting:

- If $\mathbf{x}_i$ is on right side with suffcient margin: nothing to be done
- Otherwise adjust w_j to have $\mathbf{x}_i$ better placed

NON SEPARABLE DATA: HINGE FUNCTION

Let the *hinge function* L be defined by

$$L(\mathbf{x}_i, y_i) = \max\{0, 1 - y_i(\sum_{j=1}^{d} w_j x_{ij} + b)\}$$

Partial derivatives of hinge function:

$$\frac{\partial L}{\partial w_j} = \begin{cases} 0 & \text{if } y_i(\sum_{j=1}^{d} w_j x_{ij} + b) \geq 1 \\ -y_i x_{ij} & \text{otherwise} \end{cases} \quad (22)$$

Reflecting:

- If $\mathbf{x}_i$ is on right side with suffcient margin: nothing to be done
- Otherwise adjust w_j to have $\mathbf{x}_i$ better placed

General / Further Reading

Literature

- Deep Learning, Chapter 5: https://www.deeplearningbook.org/
- Mining Massive Datasets , Chapter 12, Section 3: http://infolab.stanford.edu/~ullman/mmds/ch12.pdf