

Perceptron Classifier Empirical vs Structural Risk Minimization

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LECTURE PLAN

- The problem of classifier design.
- Empirical and structural risk.
- Perceptron algorithms.
- Optimal separating plane with the Kozinec algorithm.

Classifier Design (Bayes)



- **The object** of interest is characterised by observable properties $x \in X$ and its class membership (unobservable, hidden state) $k \in K$, where X is the space of observations and K the set of hidden states.
- The objective of classifier design is to find a strategy $q^* \colon X \to K$ that has some optimal properties.
- Bayesian decision theory solves the problem of minimisation of risk

$$R(q) = \sum_{\mathbf{x},k} p(\mathbf{x},k) W(q(\mathbf{x}),k)$$

given the following quantities:

- $p(\mathbf{x}, k), \forall \mathbf{x} \in X, k \in K$ the statistical model of the dependence of the observable properties (measurements) on class membership (almost always unknown)
- $W(q(\mathbf{x}), k)$ the loss of decision $q(\mathbf{x})$ if the true class is k

Classifier Design via Parameter Estimation

• Assume $p(\mathbf{x}, k)$ have a particular form, e.g. Gaussian (mixture), piece-wise constant, etc., with a finite (i.e. small) number of parameters θ_k .

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- igstarrow Estimate the parameters from the using training set ${\cal T}$
- Solve the classifier design problem (e.g. risk minimisation), substituting the estimated $\hat{p}(\mathbf{x}, k)$ for the true (and unknown) probabilities $p(\mathbf{x}, k)$
- ? : What estimation principle should be used?
- : There is no direct relationship between known properties of estimated $\hat{p}(\mathbf{x}, k)$ and the properties (typically the risk) of the obtained classifier $q'(\mathbf{x})$
- : If the true $p(\mathbf{x}, k)$ is not of the assumed form, $q'(\mathbf{x})$ may be arbitrarily bad, even for the asymptotic case $L \to \infty$.
- + : Implementation is often straightforward, especially if parameters θ_k for each class are assumed independent.
- + : Performance on test data can be predicted by crossvalidation.

Classifier Design via Risk Minimization



- How about constructing a 'direct' classifier (without estimating $p(\mathbf{x}, k)$?)
- Choose a class Q of decision functions (classifiers) $q: X \to K$.
- Find $q^* \in Q$ minimising some criterion function on the training set that approximates the risk R(q) (true risk is uknown).
- Empirical risk R_{emp} (training set error) minimization. True risk approximated by

$$R_{emp}(q_{\theta}(\mathbf{x})) = \frac{1}{L} \sum_{i=1}^{L} W(q_{\theta}(\mathbf{x}_i), k_i) ,$$

$$\theta^* = \operatorname*{argmin}_{\theta} R_{emp}(q_{\theta}(\mathbf{x}))$$

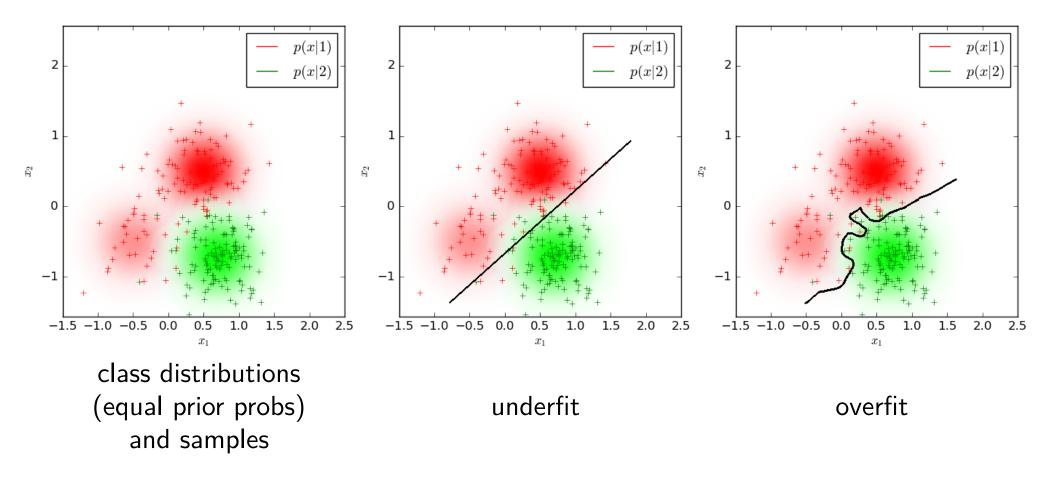
Examples: Perceptron, Neural nets (Back-propagation), etc.

Empirical Risk Minimization Can Lead To Overfitting

- How wide a class Q of classifiers $q_{\theta}(\mathbf{x})$ should be used?
- The problem of generalization is a key problem of pattern recognition: a small empirical risk R_{emp} need not imply a small true expected risk R.

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As discussed previously, a suitable model can be selected e.g. using cross-validation.

Structural Risk Minimization Principle (1)

We would like to minimise the risk

$$R(q) = \sum_{x,k} p(\mathbf{x},k) W(q_{\theta}(\mathbf{x}),k) ,$$

but $p(\mathbf{x}, k)$ is unknown.

Vapnik and Chervonenkis inequality:

$$\Pr\left(R(q) \leqslant R_{emp}(q) + \sqrt{\frac{1}{N} \left[h\left(\log\left(\frac{2N}{h}\right) + 1\right) - \log\left(\frac{\eta}{4}\right)\right]}\right) = 1 - \eta, \tag{1}$$

where N is the training set size, h is the VC dimension (capacity) of the class of strategies Q and $0 < \eta < 1$. Valid only for $h \ll N$.

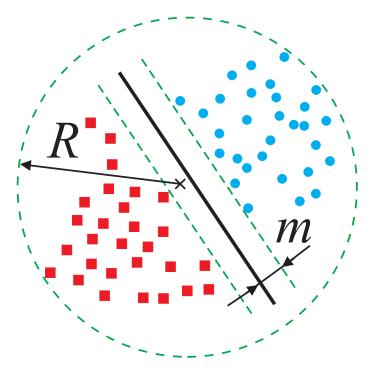
Notes:

- + the term does not depend on the unknown $p(\mathbf{x},k)$
- + VC dimension h known for some classes of Q, e.g. linear classifiers.



Structural Risk Minimization Principle (2)

There are more types of upper bounds on the expected risk. E.g. for linear discriminant functions





VC dimension (capacity)

$$h \leq \frac{R^2}{m^2} + 1$$

• Examples of learning algorithms: SVM or ε -Kozinec.

$$(\mathbf{w}^*, b^*) = \underset{\mathbf{w}, b}{\operatorname{argmax}} \min \left(\min_{x \in X_1} \frac{\mathbf{w} \cdot \mathbf{x} + b}{\|\mathbf{w}\|}, \min_{x \in X_2} - \frac{\mathbf{w} \cdot \mathbf{x} + b}{\|\mathbf{w}\|} \right)$$

Empirical Risk Minimisation, Notes



Is then empirical risk minimisation = minimisation of training set error, e.g. neural networks with backpropagation, useless? No, because:

- structural risk may be so large that the upper bound is useless.
- + Vapnik's theory justifies using empirical risk minimisation on classes of functions with finite VC dimension.
- + Vapnik suggests learning with progressively more complex classes Q.
- + Empirical risk minimisation is computationally hard (impossible for large L). Most classes of decision functions Q where empirical risk minimisation (at least local) can be efficiently organised are often useful.

Linear Classifiers



- For some statistical models, the Bayesian or non-Bayesian strategy is implemented by a linear discriminant function.
- Capacity (VC dimension) of linear strategies in an *n*-dimensional space is *n* + 2. Thus, the learning task is well-posed, i.e., strategy tuned on a finite training multiset does not differ much from correct strategy found for a statistical model.
- There are efficient learning algorithms for linear classifiers.
- Some non-linear discriminant functions can be implemented as linear after the feature space transformation.

Linear Separability (Two Classes)

Consider a dataset $\mathcal{T} = \{(\mathbf{x}_1, k_1), (\mathbf{x}_2, k_2), ..., (\mathbf{x}_L, k_L)\}$, with $\mathbf{x}_i \in \mathbb{R}^D$ and $k_i \in \{-1, 1\}$ (*i* = 1, 2, ..., *L*.)

The data are **linearly separable** if there exists a hyperplane which divides \mathbb{R}^D to two half-spaces such that the data of a given class are all in one half-space.

Formally, the data are linearly separable if

$$\exists \mathbf{w} \in \mathbb{R}^{D+1} \colon \operatorname{sign}\left(\mathbf{w} \cdot \begin{bmatrix} 1 \\ \mathbf{x}_i \end{bmatrix}\right) = k_i \quad \forall i = 1, 2, ..., L.$$
(2)

Example of linearly separable data is on the next slide.

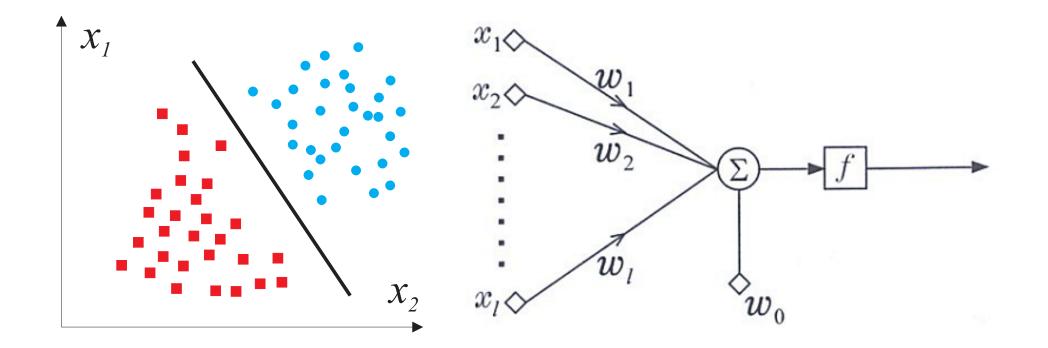


Dichotomy, Two Classes Only



|K| = 2, i.e. two hidden states (typically also classes)

$$q(x) = \begin{cases} k = 1, & \text{if } \mathbf{w} \cdot \mathbf{x} + w_0 > 0, \\ k = -1, & \text{if } \mathbf{w} \cdot \mathbf{x} + w_0 < 0. \end{cases}$$
(3)



Perceptron Classifier



Input:
$$T = \{(\mathbf{x}_1, k_1) \dots (\mathbf{x}_L, k_L)\}, \quad k \in \{-1, 1\}$$

Goal: Find a weight vector w and offset w_0 such that :

$$\mathbf{w} \cdot \mathbf{x}_j + w_0 > 0$$
 if $k_j = 1$, $(\forall j \in \{1, 2, ..., L\})$
 $\mathbf{w} \cdot \mathbf{x}_j + w_0 < 0$ if $k_j = -1$ (4)

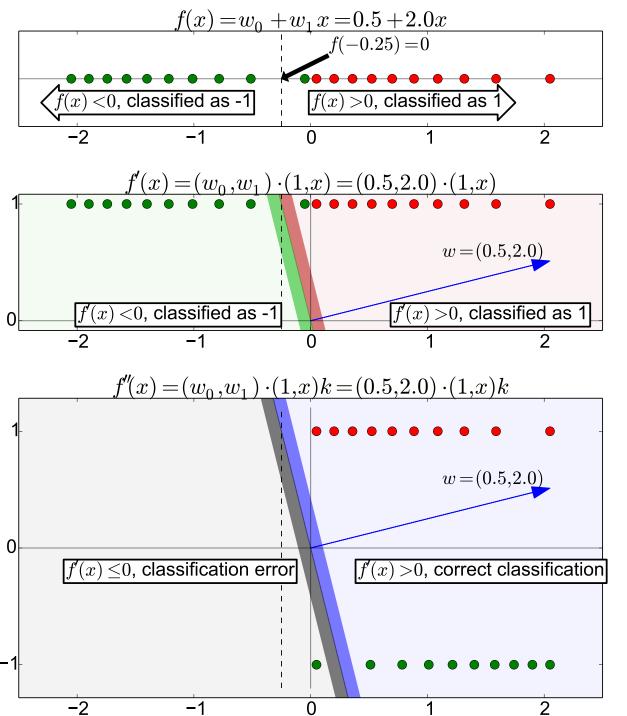
Equivalently, (as in the logistic regression lecture), with $\mathbf{x}' = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}$ and $\mathbf{w}' = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$:

$$\mathbf{w}' \cdot \mathbf{x}'_{j} > 0 \quad \text{if} \quad k_{j} = 1 \qquad (\forall j \in \{1, 2, ..., L\}),$$

$$\mathbf{w}' \cdot \mathbf{x}'_{j} < 0 \quad \text{if} \quad k_{j} = -1,$$
(5)

or, with $\mathbf{x}_{j}'' = k_{j}\mathbf{x}_{j}'$, $\mathbf{w}' \cdot \mathbf{x}_{j}'' > 0$, $(\forall j \in \{1, 2, ..., L\}.)$ (6)

Perceptron Classifier Formulation, Example





Augmenting by 1's, $\mathbf{x}'_i \in \mathbb{R}^2$

class 1,

Data points, $x \in \mathbb{R}$

Multiplying by k_j , $k_j \mathbf{x}''_j \in \mathbb{R}^2$

Perceptron Learning: Algorithm



We use the last representation $\begin{pmatrix} \mathbf{x}_{j}'' = k_{j} \begin{bmatrix} 1 \\ \mathbf{x}_{j} \end{bmatrix}$, $\mathbf{w}' = \begin{bmatrix} w_{0} \\ \mathbf{w} \end{bmatrix}$) and drop the dashes to avoid notation clutter.

Goal: Find a weight vector $\mathbf{w} \in \mathbb{R}^{D+1}$ (original feature space dimensionality is D) such that:

$$\mathbf{w} \cdot \mathbf{x}_j > 0 \qquad (\forall j \in \{1, 2, \dots, L\}) \tag{7}$$

Perceptron algorithm, (Rosenblat 1962):

- 1. t = 0, $\mathbf{w}^{(t)} = 0$.
- 2. Find a wrongly classified observation \mathbf{x}_j :

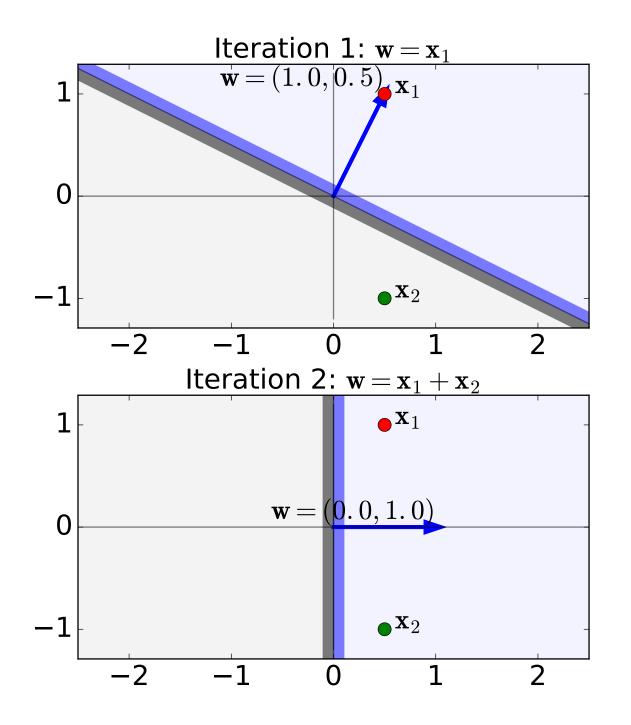
$$\mathbf{w}^{(t)} \cdot \mathbf{x}_j \le 0, \qquad (j \in \{1, 2, ..., L\}.)$$

3. If there is no misclassified observation then terminate. Otherwise,

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \mathbf{x}_j \,.$$

4. Goto 2.

Perceptron, Example 1





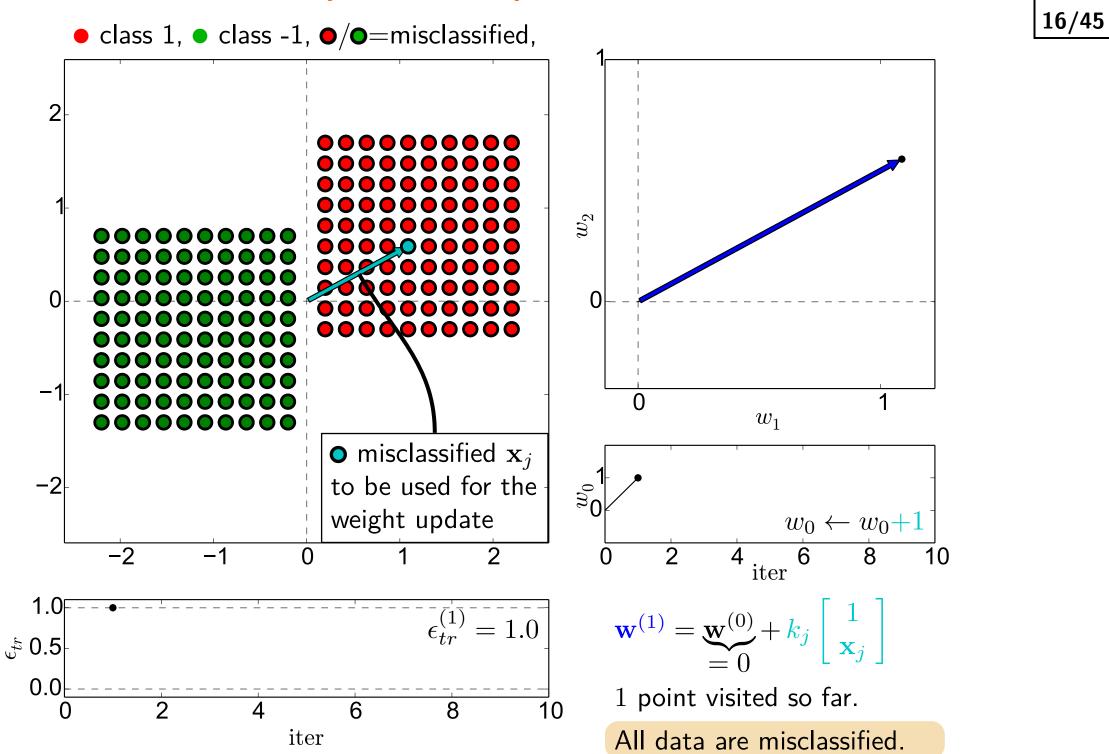
Consider this dataset with 2 points. As $\mathbf{w}^{(0)} = 0$, all points are misclassified. Order the points randomly and go over this dataset. Find the first misclassified point. It is \mathbf{x}_1 , say. Make the update of weight, $\mathbf{w}^{(1)} \leftarrow \mathbf{w}^{(0)} + \mathbf{x}_1$.

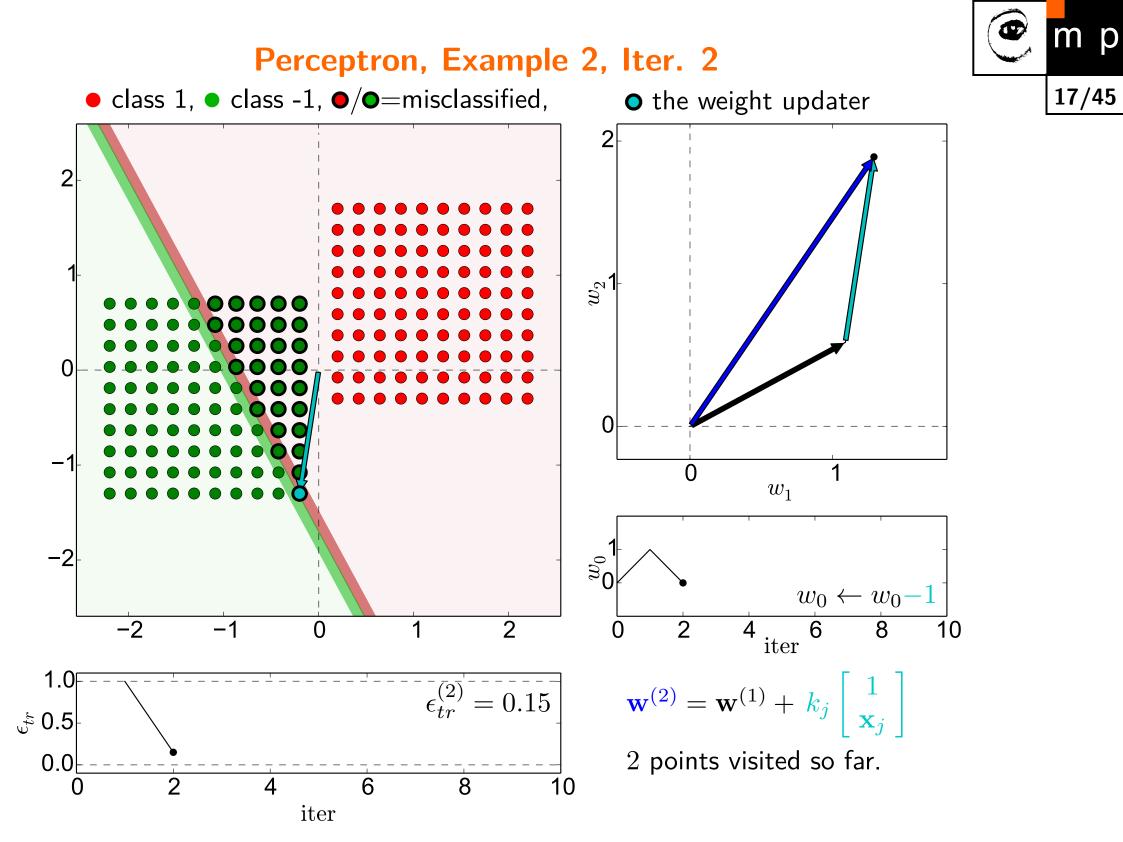
Note that \mathbf{x}_2 is misclassified.

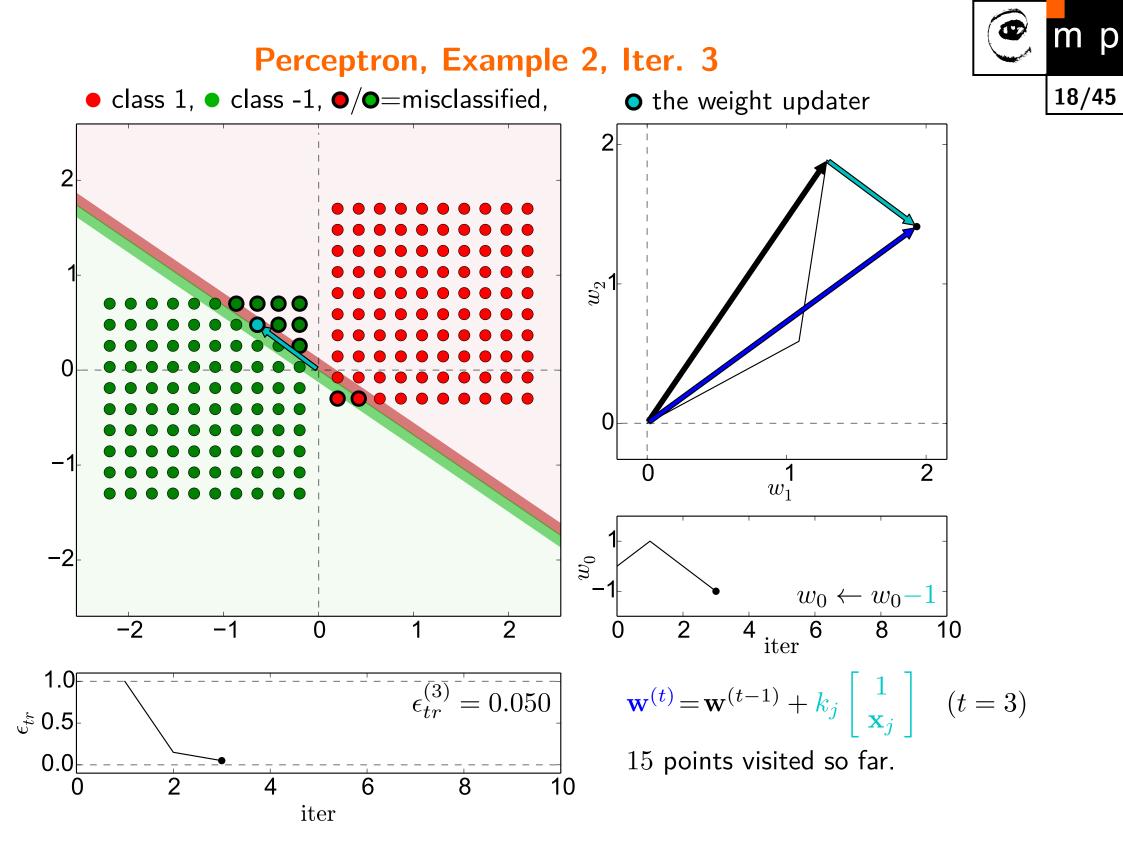
 $\mathbf{w}^{(2)} \leftarrow \mathbf{w}^{(1)} + \mathbf{x}_2$. The whole dataset is correctly classified. Done.

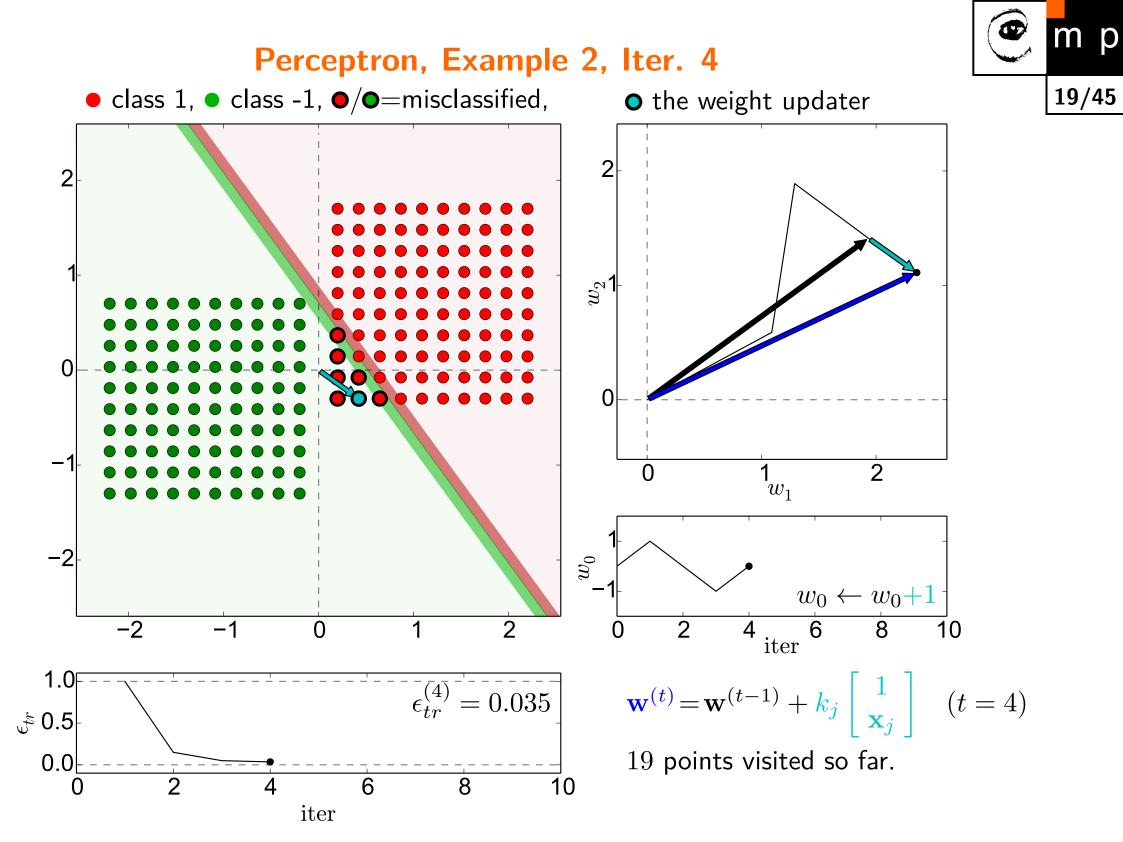
Perceptron, Example 2, Iter. 1

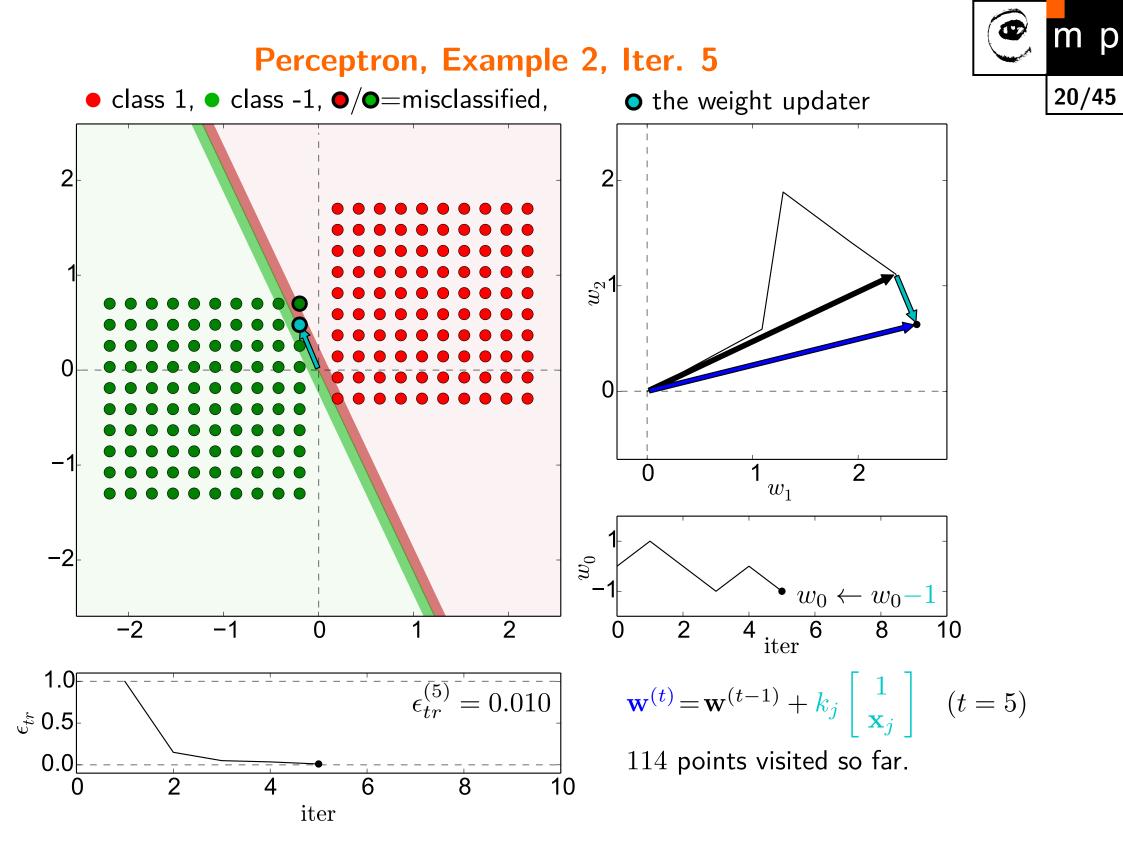
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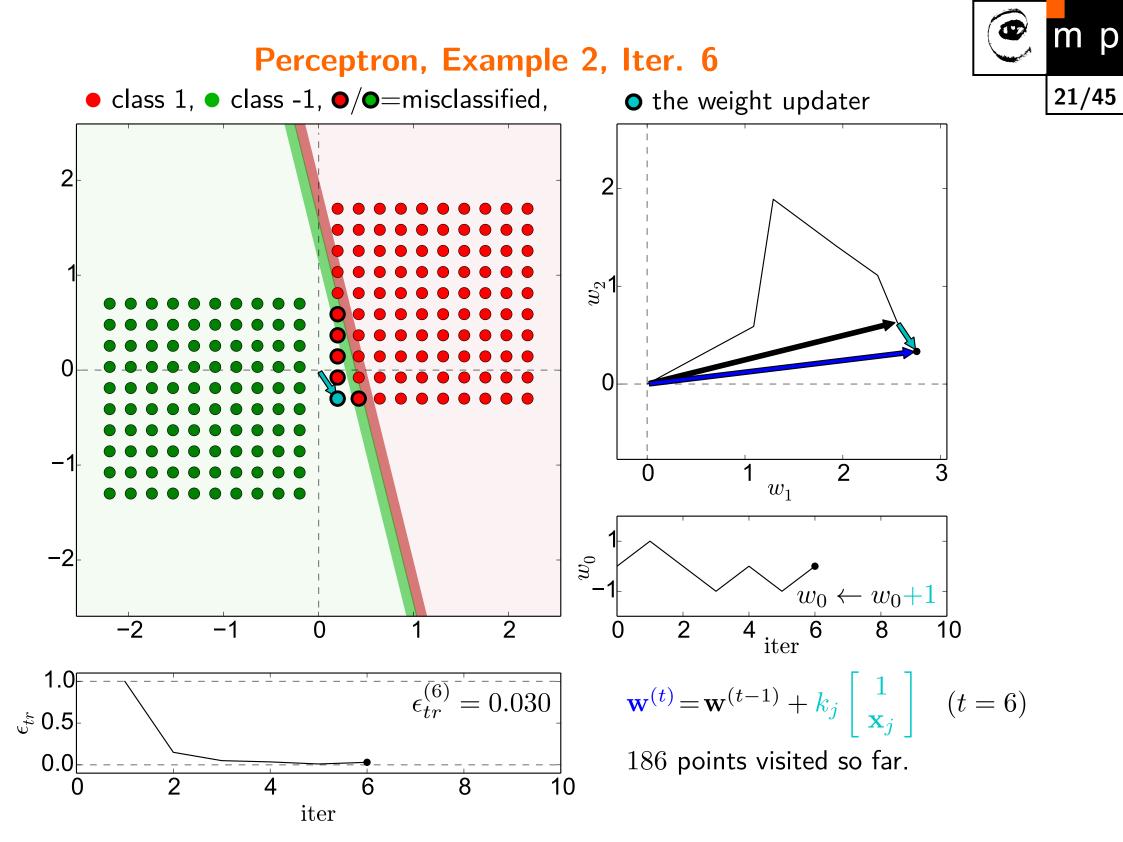








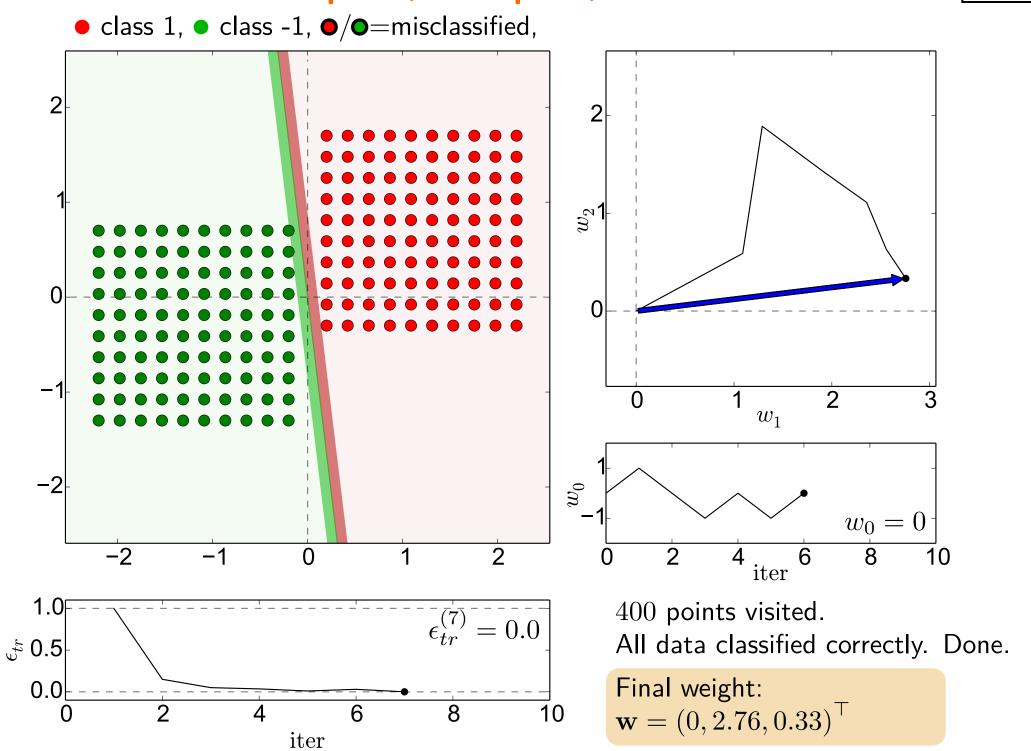




Perceptron, Example 2, Iter. 7

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Novikoff Theorem

Let the data be linearly separable and let there be a unit vector ${\bf u}$ and a scalar $\gamma\in \mathbb{R}^+$ such that

$$\mathbf{u} \cdot \mathbf{x}_j \ge \gamma \qquad \forall j \in \{1, 2, ..., L\} \qquad (\|\mathbf{u}\| = 1)$$
(8)

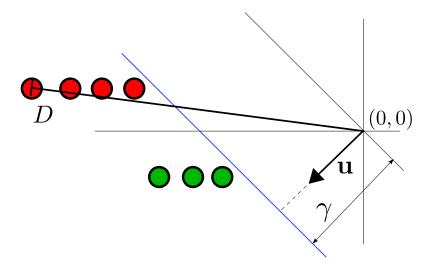
Let the norm of the longest vector in the dataset be D:

$$D = \max_{x \in \mathcal{T}} \|\mathbf{x}\|.$$
(9)

Then the perceptron algorithm will finish in a finite number of steps t^* , with

? How to terminate perceptron learning?

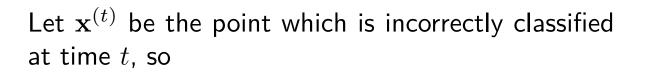




$$t^* \le \frac{D^2}{\gamma^2} \,. \tag{10}$$

Novikoff Theorem, Proof (1)

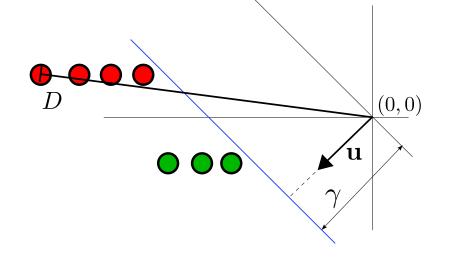




$$\mathbf{w}^{(t)} \cdot \mathbf{x}^{(t)} \le 0. \tag{11}$$

Recall that the weight $\mathbf{w}^{(t+1)}$ is computed using this update $\mathbf{x}^{(t)}$ as

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \mathbf{x}^{(t)}.$$
(12)
For the squared norm of $\mathbf{w}^{(t+1)}$, we have



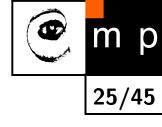
$$\|\mathbf{w}^{(t+1)}\|^2 = \mathbf{w}^{(t+1)} \cdot \mathbf{w}^{(t+1)} = (\mathbf{w}^{(t)} + \mathbf{x}^{(t)}) \cdot (\mathbf{w}^{(t)} + \mathbf{x}^{(t)})$$
(13)

$$= \|\mathbf{w}^{(t)}\|^2 + 2 \underbrace{\mathbf{w}^{(t)} \cdot \mathbf{x}^{(t)}}_{\leq 0} + \underbrace{\|\mathbf{x}^{(t)}\|^2}_{\leq D^2}$$
(14)

$$\leq \|\mathbf{w}^{(t)}\|^2 + D^2 \leq \|\mathbf{w}^{(t-1)}\|^2 + 2D^2$$
(15)

$$\leq \|\mathbf{w}^{(t-2)}\|^2 + 3D^2 \leq \dots \leq \|\mathbf{w}^{(0)}\|^2 + (t+1)D^2$$
 (16)

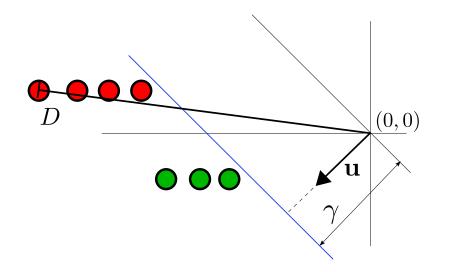
 $\|\mathbf{w}^{(t+1)}\|^2 \le (t+1)D^2 \tag{17}$



Novikoff Theorem, Proof (2)

We also have that

$$\mathbf{w}^{(t+1)} \cdot \mathbf{u} = \mathbf{w}^{(t)} \cdot \mathbf{u} + \underbrace{\mathbf{x}^{(t)} \cdot \mathbf{u}}_{\geq \gamma}$$
(18)
$$\geq \mathbf{w}^{(t)} \cdot \mathbf{u} + \gamma \geq \mathbf{w}^{(t-1)} \cdot \mathbf{u} + 2\gamma$$
(19)
$$\geq \mathbf{w}^{(t-2)} \cdot \mathbf{u} + 3\gamma \geq \dots$$
(20)
$$\geq \mathbf{w}^{(0)} \cdot \mathbf{u} + (t+1)\gamma$$
(21)



 $\mathbf{w}^{(t+1)} \cdot \mathbf{u} \geq (t+1)\gamma \tag{22}$

We take the two inequalities together, to obtain

$$(t+1)D^2 \ge \|\mathbf{w}^{(t+1)}\|^2 \ge (\mathbf{w}^{(t+1)} \cdot \mathbf{u})^2 \ge (t+1)^2 \gamma^2 \qquad (\|\mathbf{u}\| = 1)$$
 (23)

Therefore,

$$(t+1) \le \frac{D^2}{\gamma^2} \,. \tag{24}$$

Perceptron Learning as an Optimisation Problem (1)

Perceptron algorithm, batch version, handling non-separability, another perspective:

Input: $\mathcal{T} = {\mathbf{x}_1, \dots \mathbf{x}_L}$ **Output**: a weight vector \mathbf{w} minimising

$$J(\mathbf{w}) = |\{\mathbf{x} \in X \colon \mathbf{w}^{(t)} \cdot \mathbf{x} \le 0\}|$$
(25)

or, equivalently

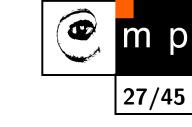
$$J(\mathbf{w}) = \sum_{\substack{\mathbf{x} \in X\\ \mathbf{w}^{(t)} \cdot \mathbf{x} \le 0}} 1$$
 (26)

What would the most common optimisation method, i.e. gradient descent, perform?

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla J(\mathbf{w}) \tag{27}$$

The gradient of $J(\mathbf{w})$ is, however, either 0 or undefined. The gradient minimisation cannot proceed.





Perceptron Learning as an Optimisation Problem (2)

Let us redefine the cost function:

$$J_{p}(\mathbf{w}) = \sum_{\substack{\mathbf{x} \in X \\ \mathbf{w} \cdot \mathbf{x} \leq 0}} (-\mathbf{w} \cdot \mathbf{x})$$
(28)
$$\nabla J_{p}(\mathbf{w}) = \frac{\partial J}{\partial \mathbf{w}} = \sum_{\substack{\mathbf{x} \in X \\ \mathbf{w} \cdot \mathbf{x} \leq 0}} (-\mathbf{x})$$
(29)

- The Perceptron Algorithm is a gradient **descent** method for J_p(w) (gradient for a single misclassified sample is -x, so the weight update is x)
- Learning and empirical risk minimisation is just an instance of an optimization problem.
- Either gradient minimisation (backpropagation in neural networks) or convex (quadratic) minimisation (in mathematical literature called convex programming) is used.

Perceptron Learning: Non-Separable Case

Perceptron algorithm, batch version, handling non-separability:

Input: $\mathcal{T} = \{\mathbf{x}_1, \dots \mathbf{x}_L\}$ Output: weight vector \mathbf{w}^*

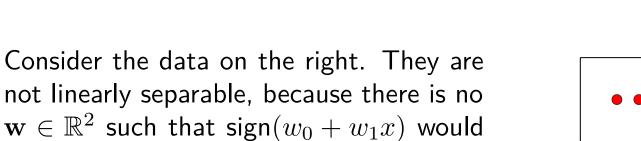
- 1. $\mathbf{w}^{(0)} = 0$, E = |T| = L, $\mathbf{w}^* = 0$.
- 2. Find all mis-classified observations $X^- = {\mathbf{x} \in X : \mathbf{w}^{(t)} \cdot \mathbf{x} \le 0}.$
- 3. if $|X^{-}| < E$ then $E = |X^{-}|$; $\mathbf{w}^{*} = \mathbf{w}^{(t)}$
- 4. if TermCond(\mathbf{w}^*, t, t_{lup}) then terminatate (t_{lup} is the time of the last update) else:

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \eta_t \sum_{x \in X^-} x$$

- 5. Goto 2.
- The algorithm converges with probability 1 to the optimal solution.
- Convergence rate is not known.
- Termination condition TermCond(\cdot) is a complex function of the quality of the best solution, time since last update $t t_{lup}$ and requirements on the solution.



Dimension Lifting



Let us artificially enlarge the dimensionality of the feature space by a mapping $\phi(x): \mathbb{R} \to \mathbb{R}^2$:

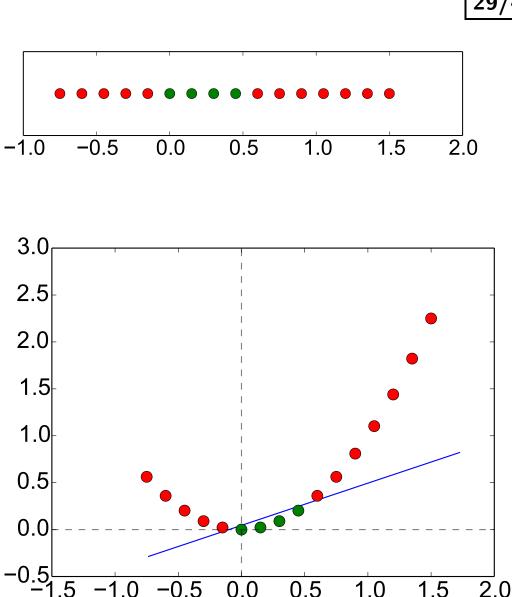
correctly classify the data.

$$\mathbf{x} \leftarrow \phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix}$$
 (30)

After such mapping, the data become linearly separable (the separator is shown on the right).

In general, lifting the feature space means adding D' dimensions and replacing the original feature vectors by

$$\mathbf{x} \leftarrow \phi(\mathbf{x}), \quad \phi(\mathbf{x}) \colon \mathbb{R}^D \to \mathbb{R}^{D+D'}.$$
 (31)





Lifting, Example 1

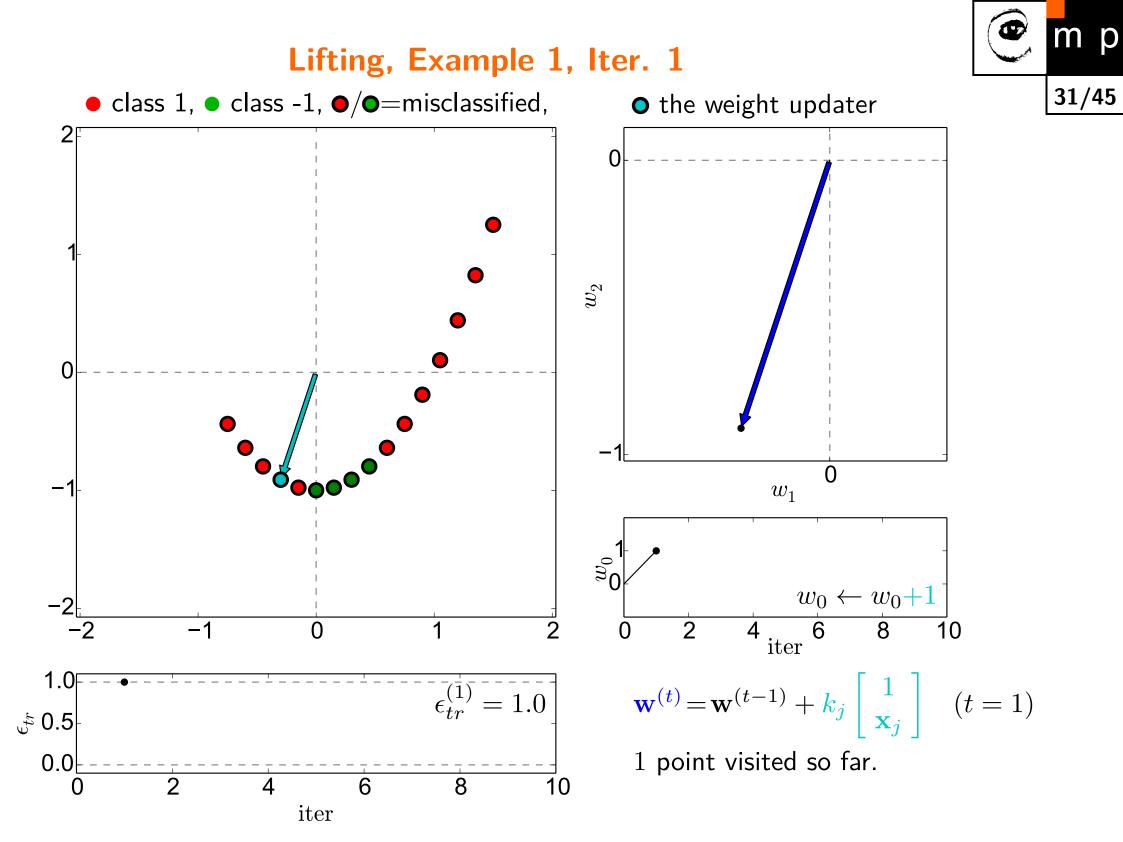
We will now apply the perceptron algorithm to the problem just shown. Note that instead of the lifting

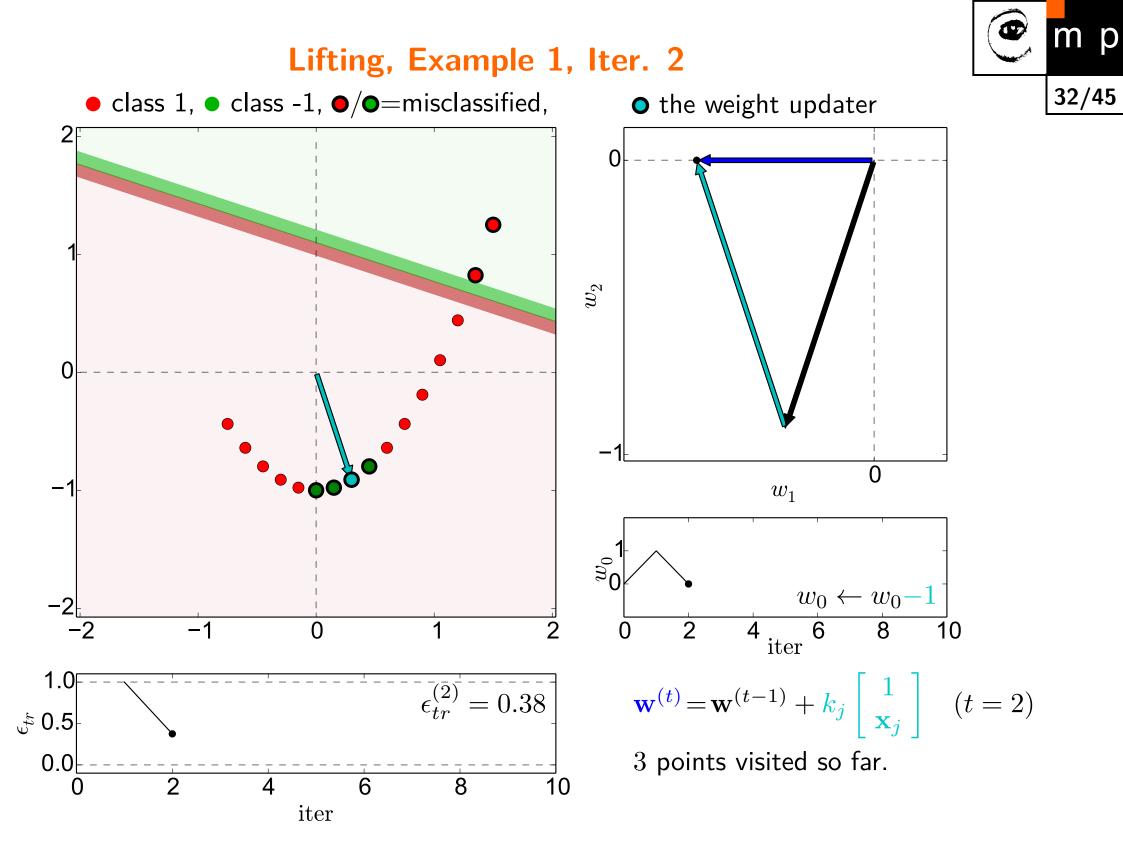
we will use

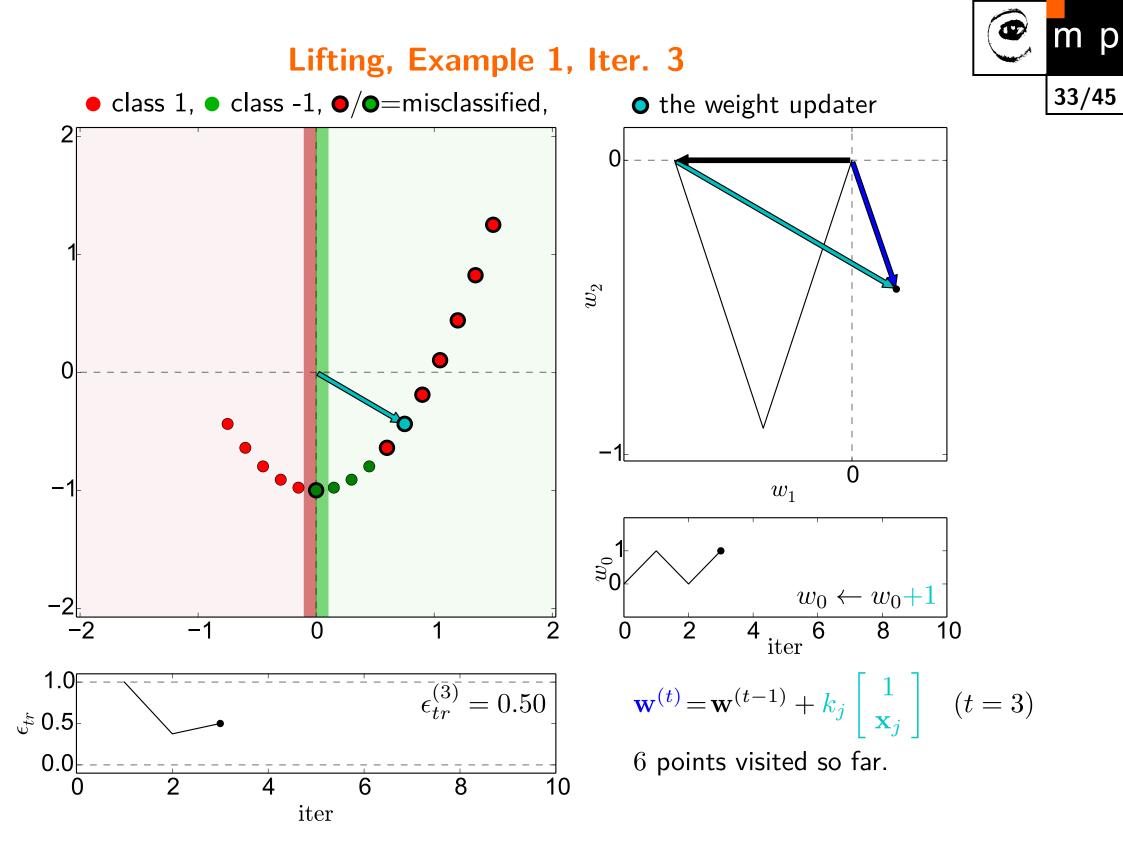
because perceptron then converges faster for our data (this is related to the Novikoff theorem.)

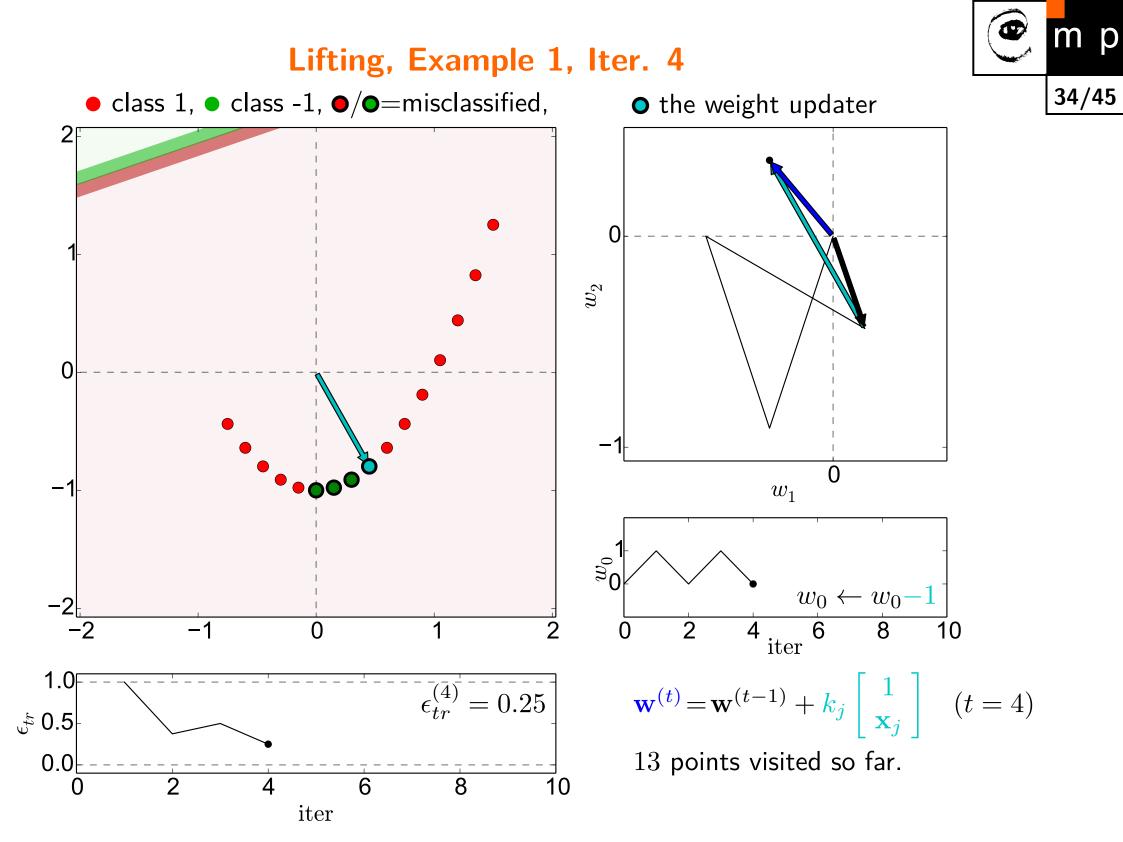
$$\mathbf{x} \leftarrow \begin{bmatrix} x\\ x^2 \end{bmatrix}$$
$$\mathbf{x} \leftarrow \begin{bmatrix} x\\ x^2 - 1 \end{bmatrix}$$

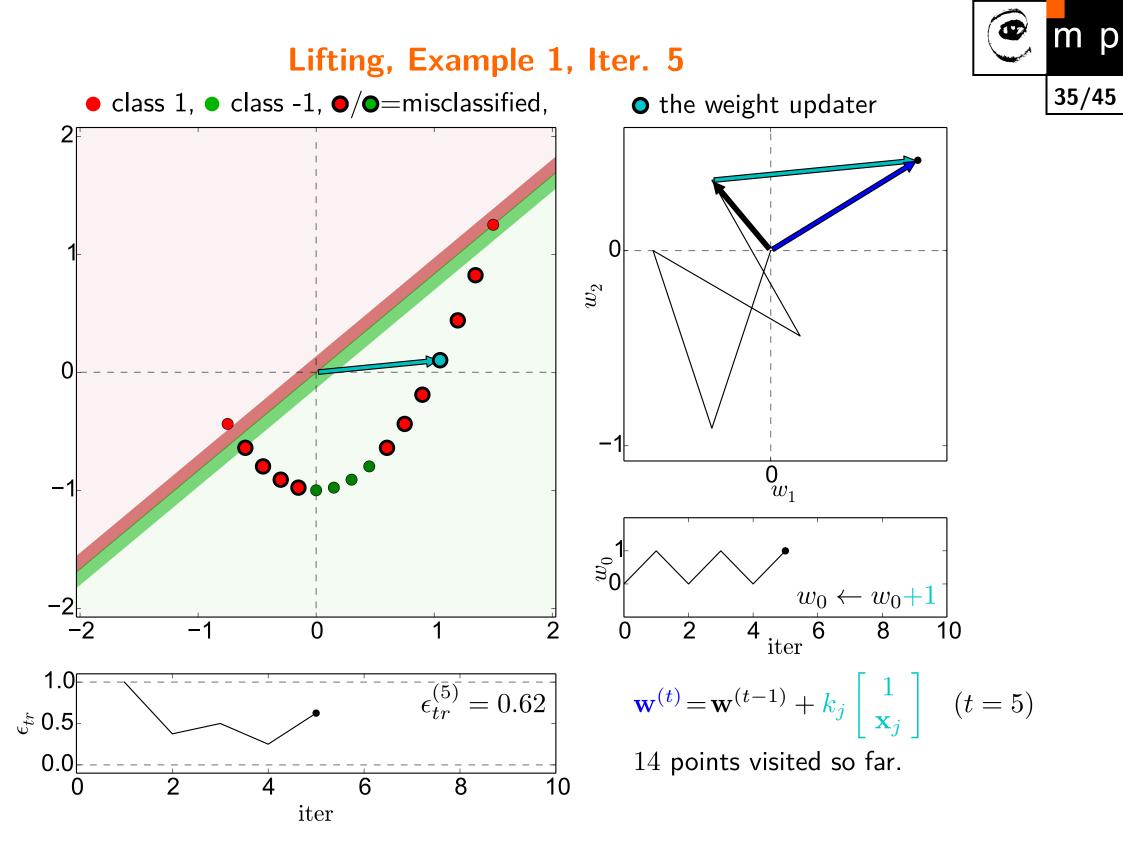


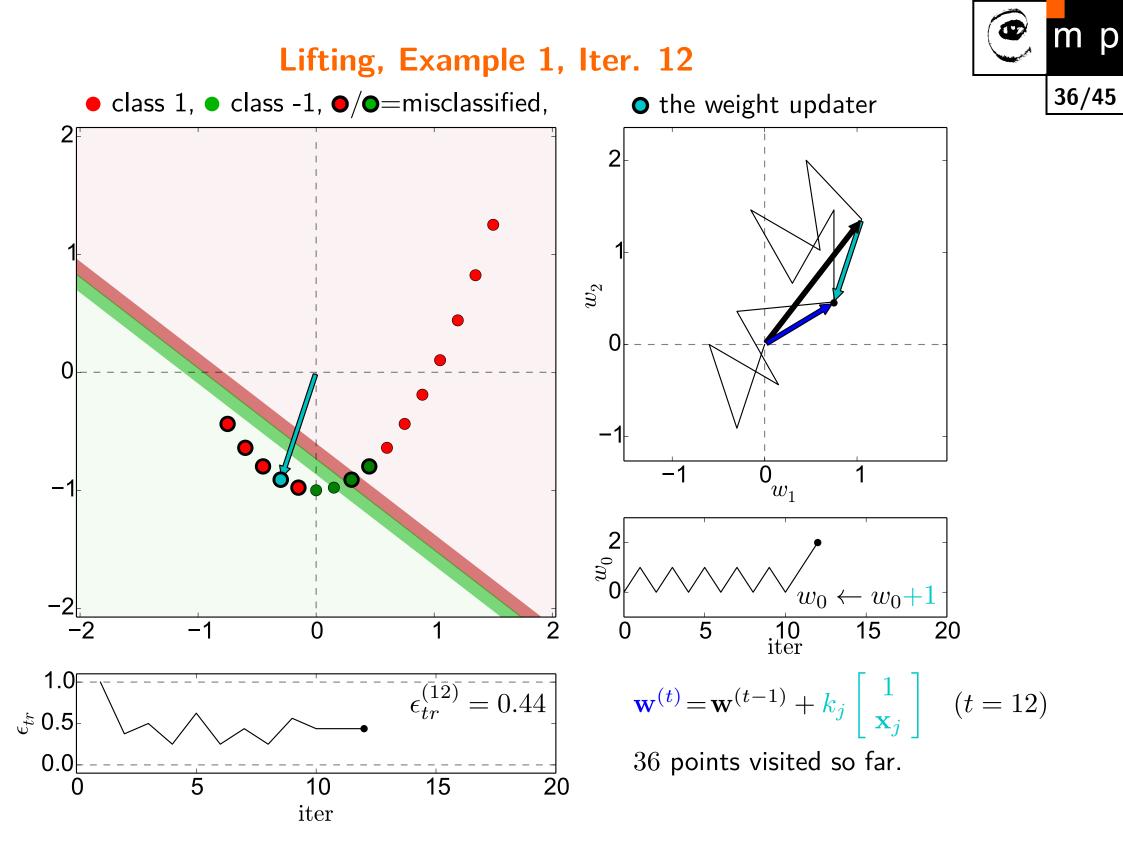


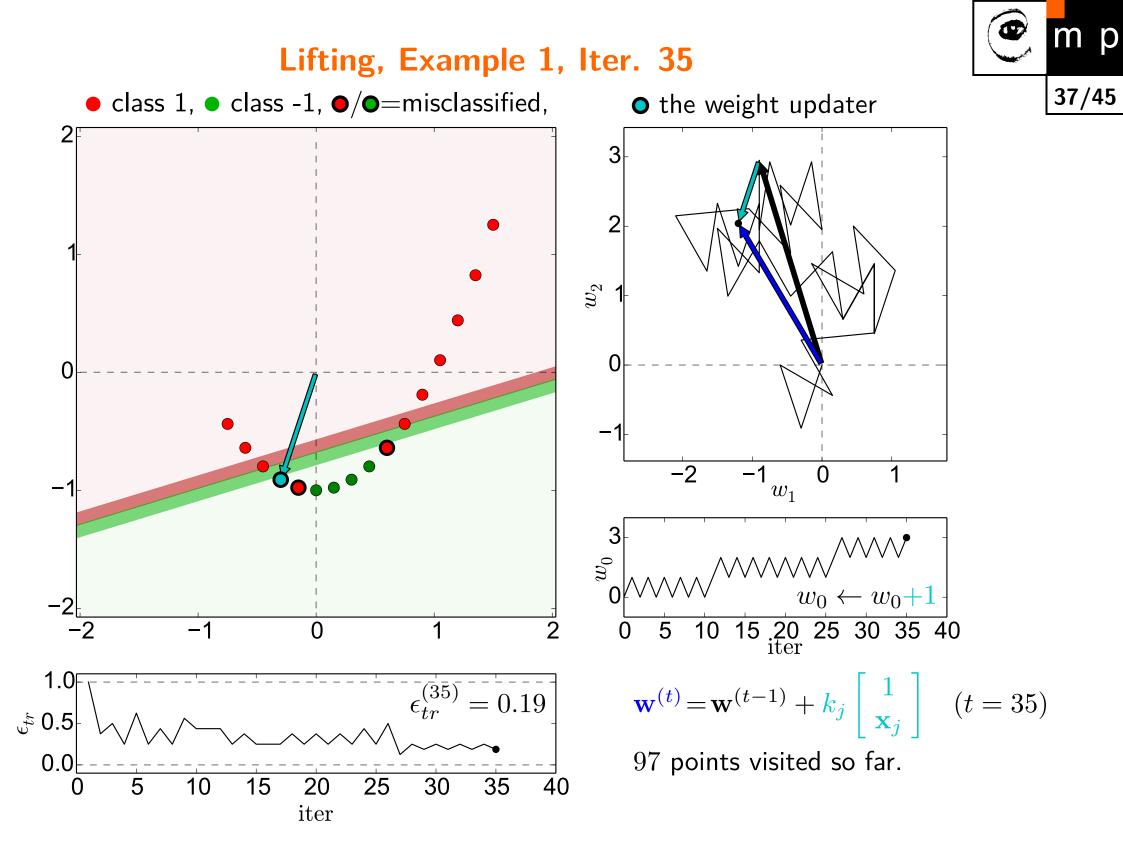


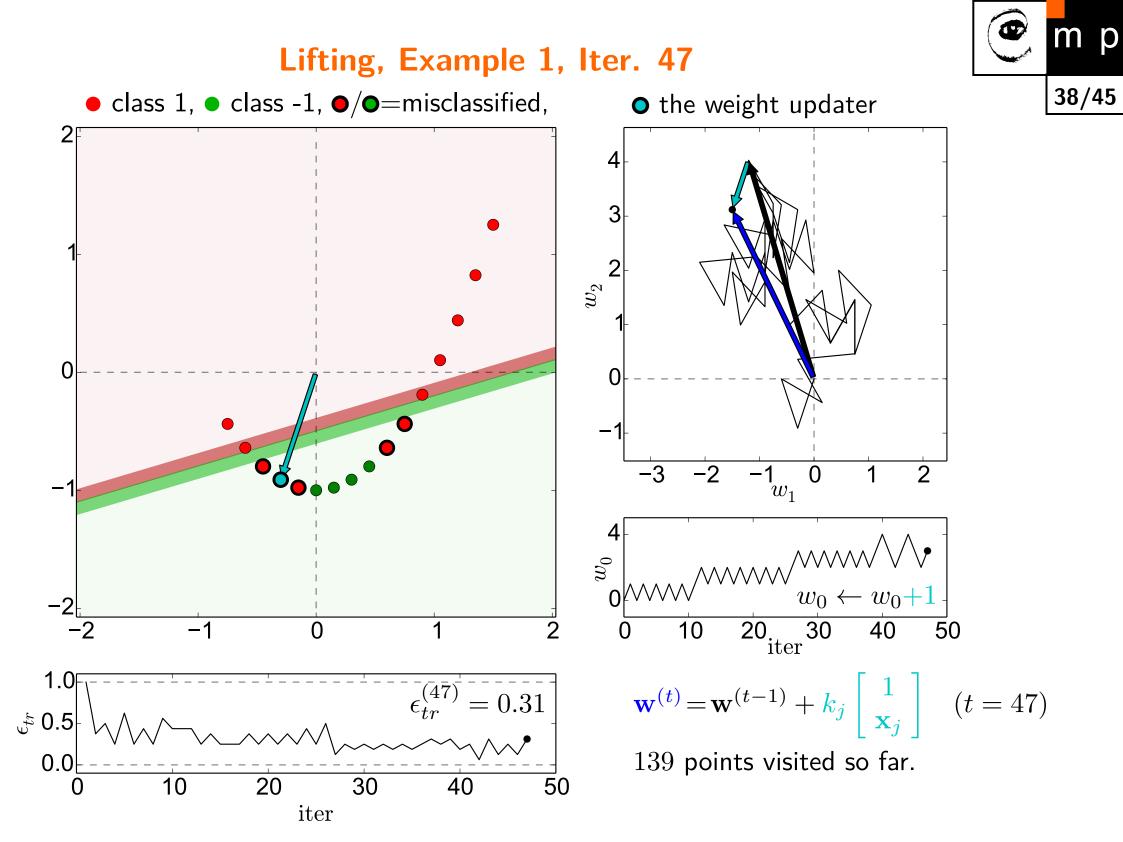


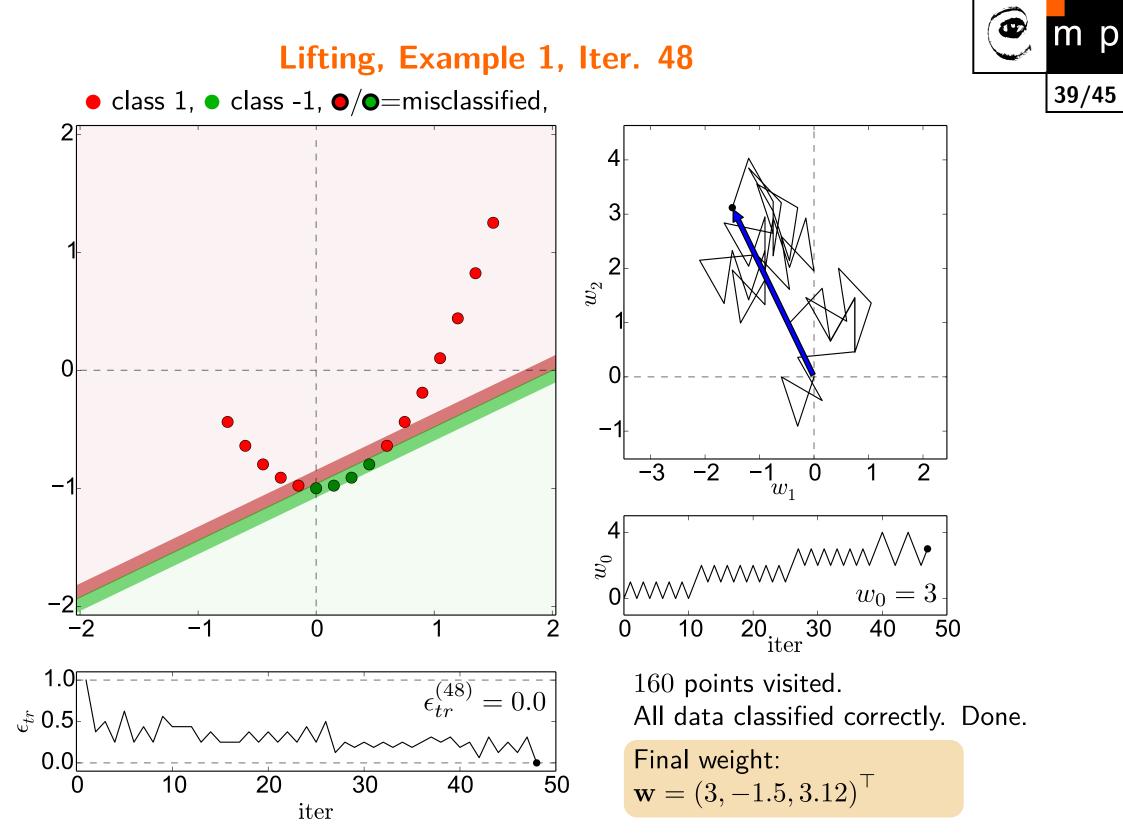




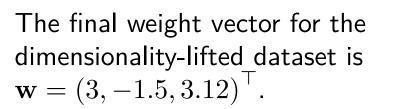






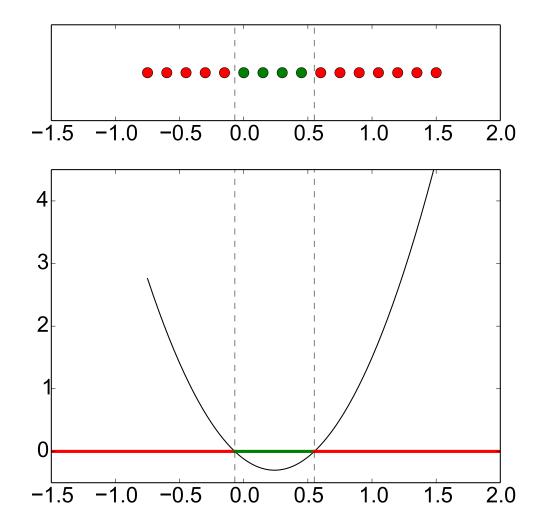


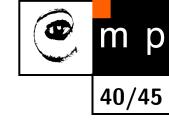
Lifting, Example 1, Result

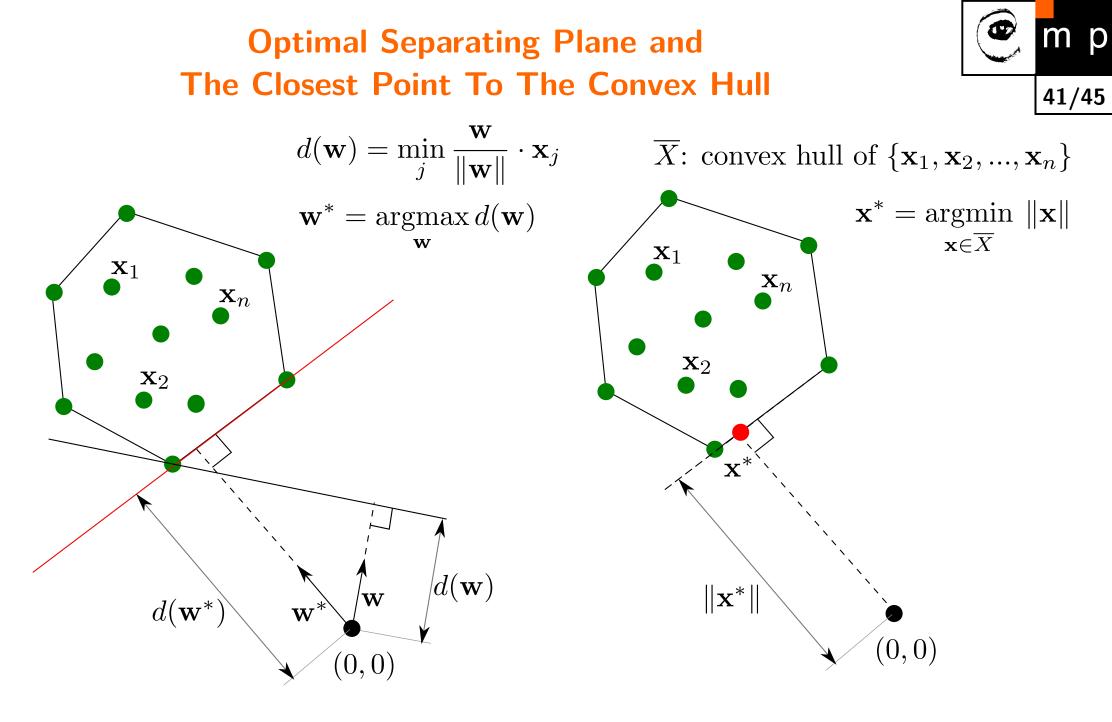


The resulting discriminant function is:

$$f(x) = 3 - 1.5x + 3.12(x^2 - 1)$$
(32)
= -0.12 - 1.5x + 3.12x². (33)



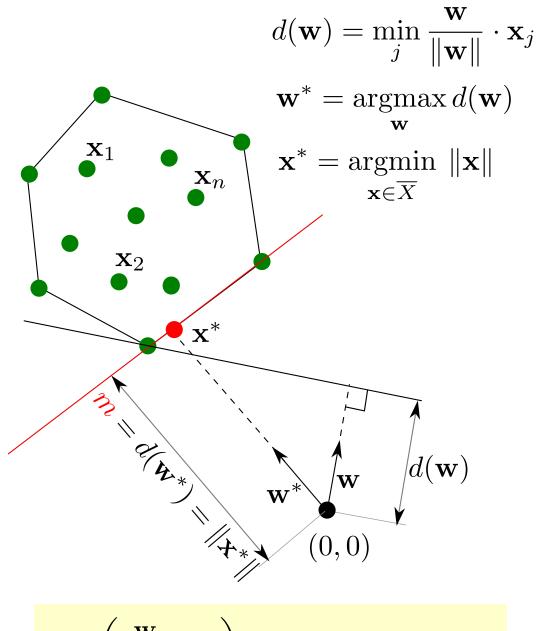




The problem of finding optimal separating hyperplane (left) is equivalent to finding closest point in the convex hull (right). Recall that the classifier that maximises separation minimises the structural risk.

Bounds For Margin m





$$\min_{j} \left(\frac{\mathbf{w}}{\|\mathbf{w}\|} \cdot \mathbf{x}_{j} \right) \le m \le \|\mathbf{w}\|, \ \mathbf{w} \in \overline{X}$$

(34)

ε -Solution

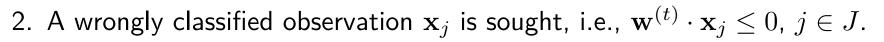


- The aim is to speed up the algorithm.
- The allowed uncertainty ε is introduced.

$$\|\mathbf{w}\| - \min_{j} \left(\frac{\mathbf{w}}{\|\mathbf{w}\|} \cdot \mathbf{x}_{j} \right) \le \varepsilon$$

Training Algorithm 2 – Kozinec (1973)

1. $\mathbf{w}^{(0)} = \mathbf{x}_j$, i.e. any observation.

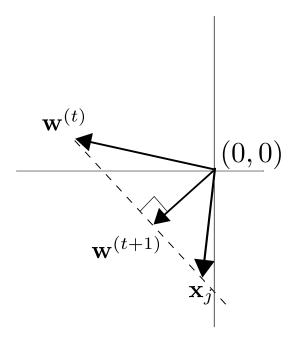


3. If there is no wrongly classified observation then the algorithm finishes otherwise

$$\mathbf{w}^{(t+1)} = (1 - \kappa^*) \, \mathbf{w}^{(t)} + \kappa^* \, \mathbf{x}_j,$$

$$\kappa^* = \operatorname*{argmin}_{\kappa \in (0,1)} \| (1 - \kappa) \, \mathbf{w}^{(t)} + \kappa \, \mathbf{x}_j \|$$

4. Goto 2.





Kozinec and ε -Solution

The second step of Kozinec algorithm is modified to:

A wrongly classified observation \mathbf{x}_j is sought for which

$$|\mathbf{w}^{(t)}| - \min_{j} \left(\frac{\mathbf{w}^{(t)}}{|\mathbf{w}^{(t)}|} \cdot \mathbf{x}_{j} \right) \ge \varepsilon$$

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