Support Vector Machines. Logistic Regression.

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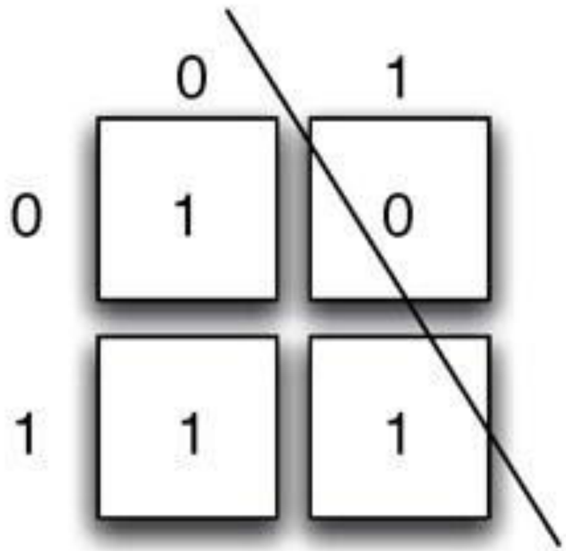
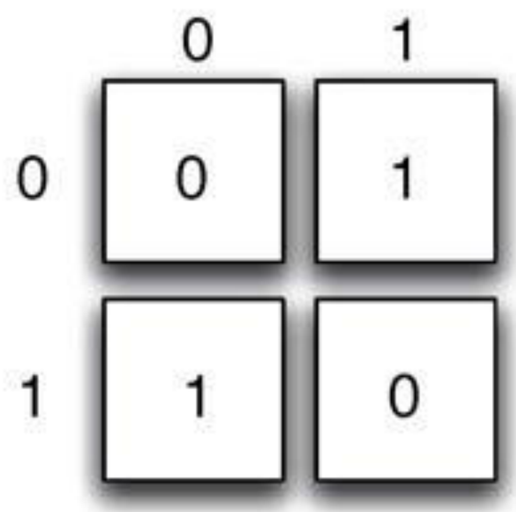
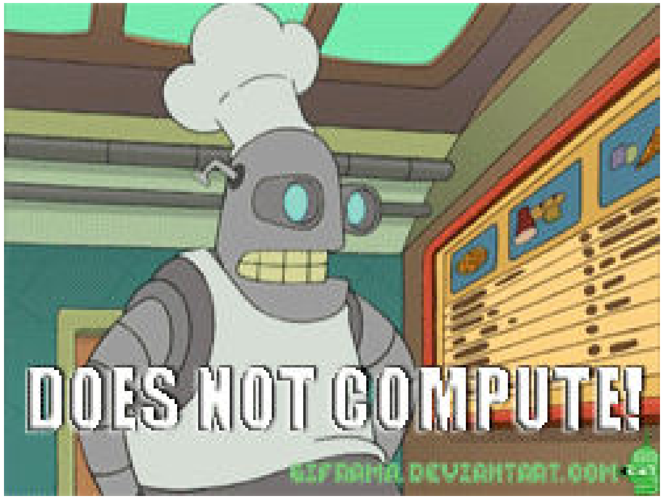
XOR (Minsky & Papert, 1969)

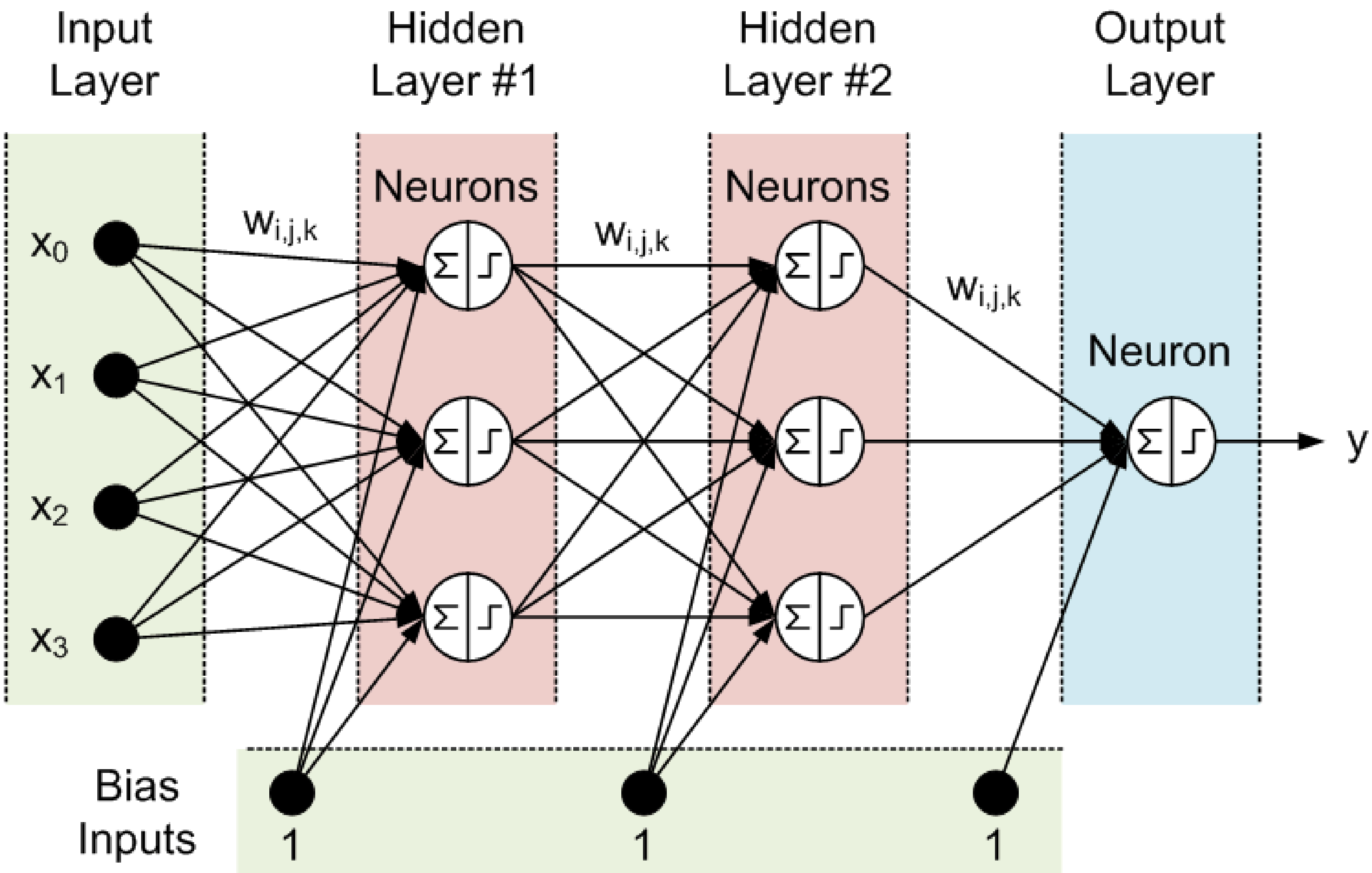
- A linear classification method cannot solve the XOR problem







Solution 1: Neural Networks



Solution 2: Kernel Methods

- Kernel methods are based on two steps:
  - ➢ 1. Embed data in a higher-dimensional Hilbert space
  - ➢ 2. Search for linear relations in the embedding space
- The embedding can be performed implicitly, by specifying the scalar product among data samples
  - ➢ Steps 1 and 2 can be comprised in one step!

Primal Form

Features: f_1, f_2, f_3, f_4, f_5, f_6, f_7

Train samples: x_1, x_2, x_3, x_4

	f_1	f_2	f_3	f_4	f_5	f_6	f_7
x_1	4	0	2	5	3	0	1
x_2	0	0	1	3	4	0	2
x_3	2	1	0	0	1	2	5
x_4	1	3	0	1	0	1	2

= **X**

l_1	1
l_2	1
l_3	-1
l_4	-1

= **L**

Linear classifier: C = (w_1, w_2, w_3, w_4, w_5, w_6, w_7, b) such that sign(X * W' + b) = L

Test samples: y_1, y_2, y_3

	f_1	f_2	f_3	f_4	f_5	f_6	f_7
y_1	1	0	2	4	2	0	2
y_2	1	2	0	1	2	2	1
y_3	3	1	0	0	4	1	1

= **Y**

p_1	?
p_2	?
p_3	?

= **P**

Apply C to obtain predictions: P = sign(Y * W' + b)

Dual form

Kernel type: **linear**

Train samples:
x_1, x_2, x_3, x_4

$$\begin{array}{c|cccc|} & x_1 & x_2 & x_3 & x_4 \\ \hline x_1 & 55 & 31 & 16 & 11 \\ x_2 & 31 & 30 & 14 & 7 \\ x_3 & 16 & 14 & 35 & 17 \\ x_4 & 11 & 7 & 17 & 16 \\ \hline \end{array} = \mathbf{X * X' = K_X}$$

$$\begin{array}{c|c|} l_1 & 1 \\ l_2 & 1 \\ l_3 & -1 \\ l_4 & -1 \\ \end{array} = \mathbf{L}$$

Linear classifier: C = $(\alpha_1, \alpha_2, \alpha_3, \alpha_4, b)$ such that $\text{sign}(K_X * \alpha' + b) = L$

Test samples:
y_1, y_2, y_3

$$\begin{array}{c|cccc|} & x_1 & x_2 & x_3 & x_4 \\ \hline y_1 & 36 & 26 & 14 & 9 \\ y_2 & 16 & 13 & 15 & 12 \\ y_3 & 25 & 18 & 18 & 9 \\ \hline \end{array} = \mathbf{Y * X' = K_Y}$$

$$\begin{array}{c|c|} p_1 & ? \\ p_2 & ? \\ p_3 & ? \\ \end{array} = \mathbf{P}$$

Apply C to obtain predictions: $P = \text{sign}(K_Y * \alpha' + b)$

Data normalization

- In primal form:

$$x \longmapsto \phi(x) \longmapsto \frac{\phi(x)}{\|\phi(x)\|}$$

- In dual form:

$$\hat{k}(x_i, x_j) = \frac{k(x_i, x_j)}{\sqrt{k(x_i, x_i) \cdot k(x_j, x_j)}}$$

- Directly on the kernel matrix:

$$\hat{K}_{ij} = \frac{K_{ij}}{\sqrt{K_{ii} \cdot K_{jj}}}$$

Data normalization (Python)

```
% X - data (one sample per row)

% L2 norm in primal form:
norms = np.linalg.norm(X, axis = 1, keepdims = True)
X = X / norms

% L2 norm in dual form:
K = np.matmul(X, X.T)
KNorm = np.sqrt(np.diag(K))
KNorm = KNorm[np.newaxis]
K = K / np.matmul(KNorm.T, KNorm)
```

How do we separate these points optimally?

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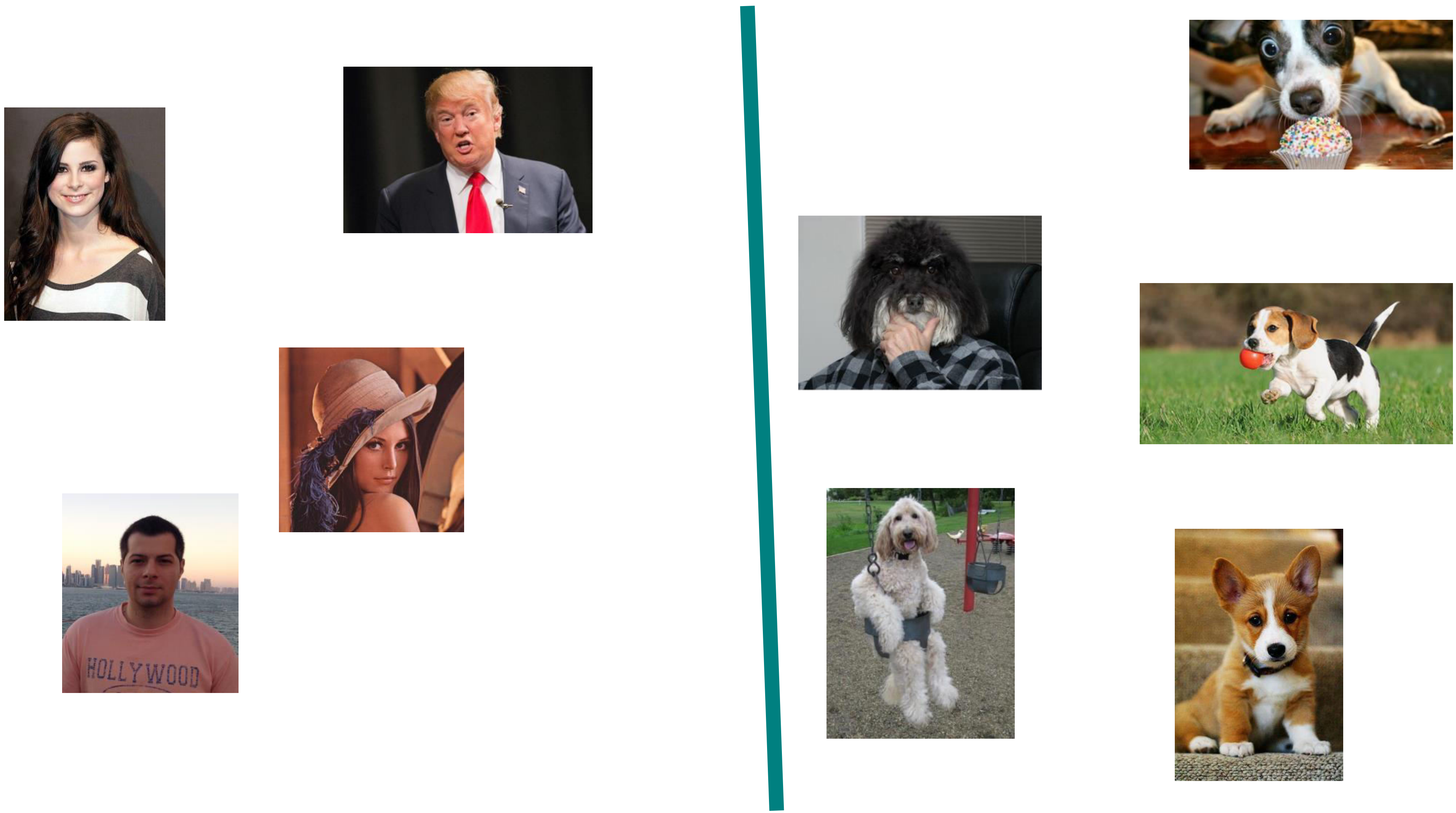
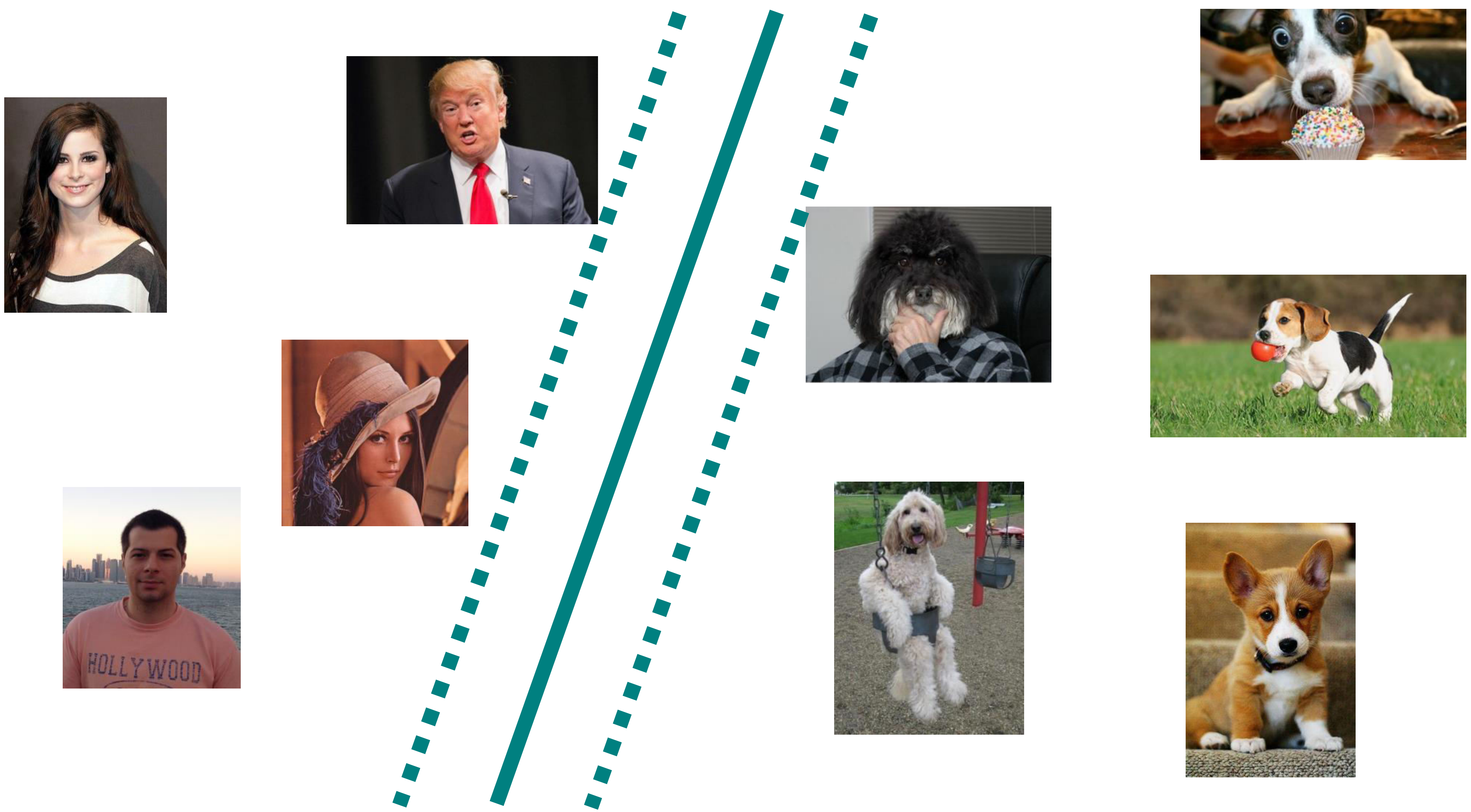


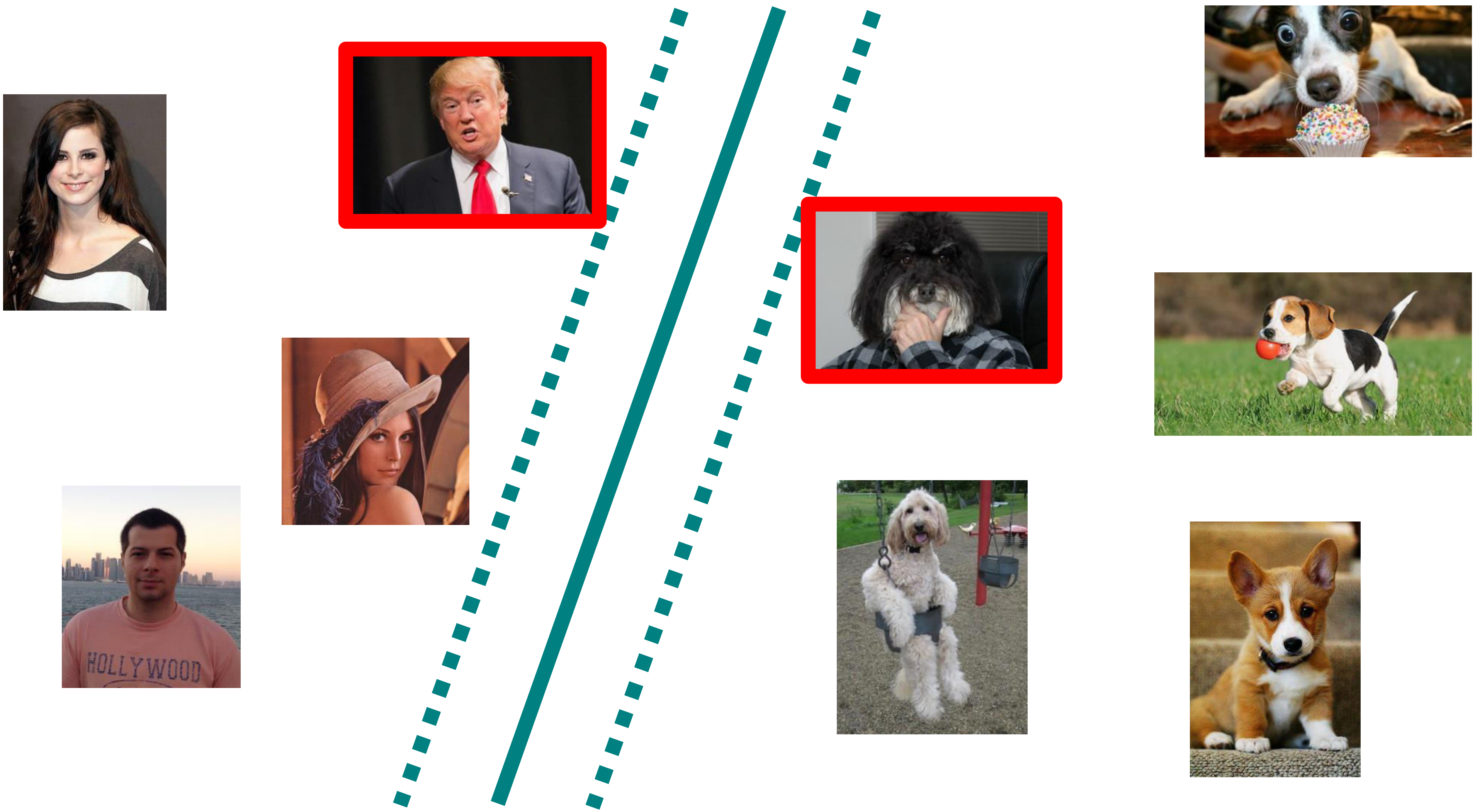
How do we separate these points optimally?

Pick the maximum margin hyperplane



Pick the maximum margin hyperplane

- Support Vector Machines (SVM)



SVM (Hard Margin)

$$S = \{(\mathbf{x_1}, y_1), (\mathbf{x_2}, y_2), \ldots, (\mathbf{x}_\ell, y_\ell)\}$$

$$g(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

$$\max_{\mathbf{w}, b, \gamma} \gamma$$

subject to

$$y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq \gamma$$

$$i = 1, \ldots, \ell$$

$$\|\mathbf{w}\|^2 = 1$$

$\Longleftrightarrow$

$$\min_{\mathbf{w}, b} \|\mathbf{w}\|^2$$

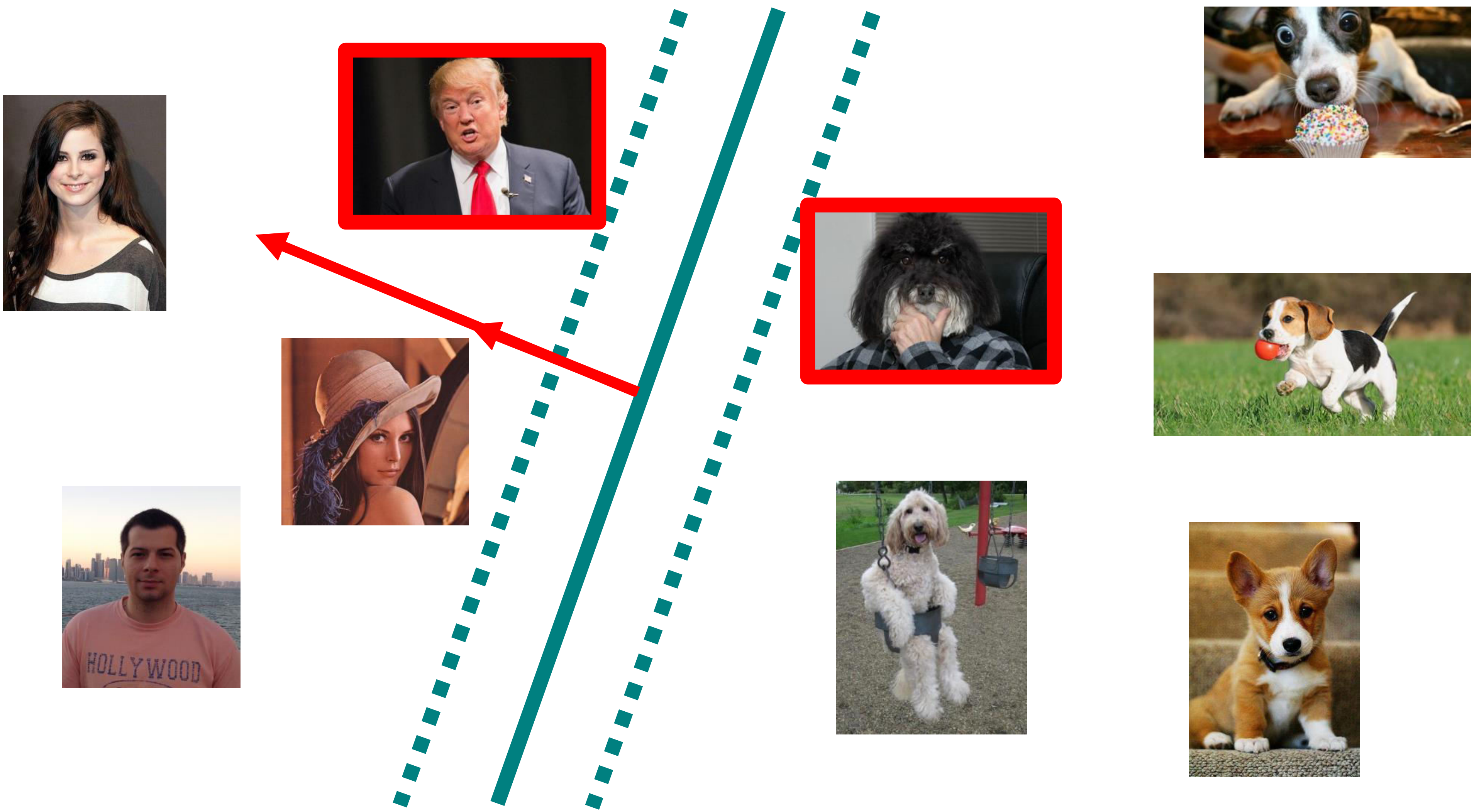
subject to

$$y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$$

$$i = 1, \ldots, \ell$$

Pick the maximum margin hyperplane

- Support Vector Machines (SVM)



SVM Dual (Hard Margin)

- Lagrange multipliers: a way of finding the extremum of a function subject to constraints
- We want to minimize $\|w\|^2$ subject to $y_i(\langle w, x_i \rangle + b) - 1 \geq 0$
- We define a new function and find its minimum instead

$$L(w, b, \alpha) = \|w\|^2 - \sum_i \alpha_i [y_i(\langle w, x_i \rangle + b) - 1], \alpha_i \geq 0$$

$$\frac{\partial L}{\partial w} = w - \sum_i \alpha_i y_i x_i = 0 \Rightarrow w = \sum_i \alpha_i y_i x_i$$

$$\frac{\partial L}{\partial b} = -\sum_i \alpha_i y_i = 0 \Rightarrow \sum_i \alpha_i y_i = 0$$

- α_i are called Lagrange multipliers

SVM Dual (Hard Margin)

$$\left.\begin{aligned} &L = \|w\|^2 - \textstyle\sum_i \alpha_i [y_i(\langle w, x_i \rangle + b) - 1] \\ &w = \textstyle\sum_i \alpha_i y_i x_i \\ &\textstyle\sum_i \alpha_i y_i = 0 \end{aligned}\right\} L = \sum_i \alpha_i - \sum_i \sum_j \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

- Note: The optimization depends only on the scalar product of training sample pairs
- α_i will be non-zero only for support vectors
- Our decision rule (in primal form) was: x is positive if $\langle w, x \rangle + b \geq 0$
- In dual form, it becomes: $\sum_i \alpha_i y_i \langle x_i, x \rangle + b \geq 0$
- Note: The decision also depends on the scalar product
- Note: b can be computed from $\sum_i \alpha_i y_i \langle x_i, x_+ \rangle + b = 1$, for some positive support vector x_+

SVM Dual (Hard Margin)

- The decision rule (in dual form) is:

x is positive if $\sum_i \alpha_i y_i \langle x_i, x \rangle + b \geq 0$

- In order to obtain α_i and b, we have to:

$$min \sum_i \alpha_i - \sum_i \sum_j \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

$$subject\ to\ \alpha_i \geq 0, \forall i$$

SVM (Hard Margin)

Primal form

- Decision rule:

$$\langle w, x \rangle + b \geq 0$$

- Optimization problem:

$$min \|w\|^2$$

$$subject\ to\ y_i(\langle w, x_i \rangle + b) - 1 \geq 0$$

Dual form

- Decision rule:

$$\sum_i \alpha_i y_i \langle x_i, x \rangle + b \geq 0$$

- Optimization problem:

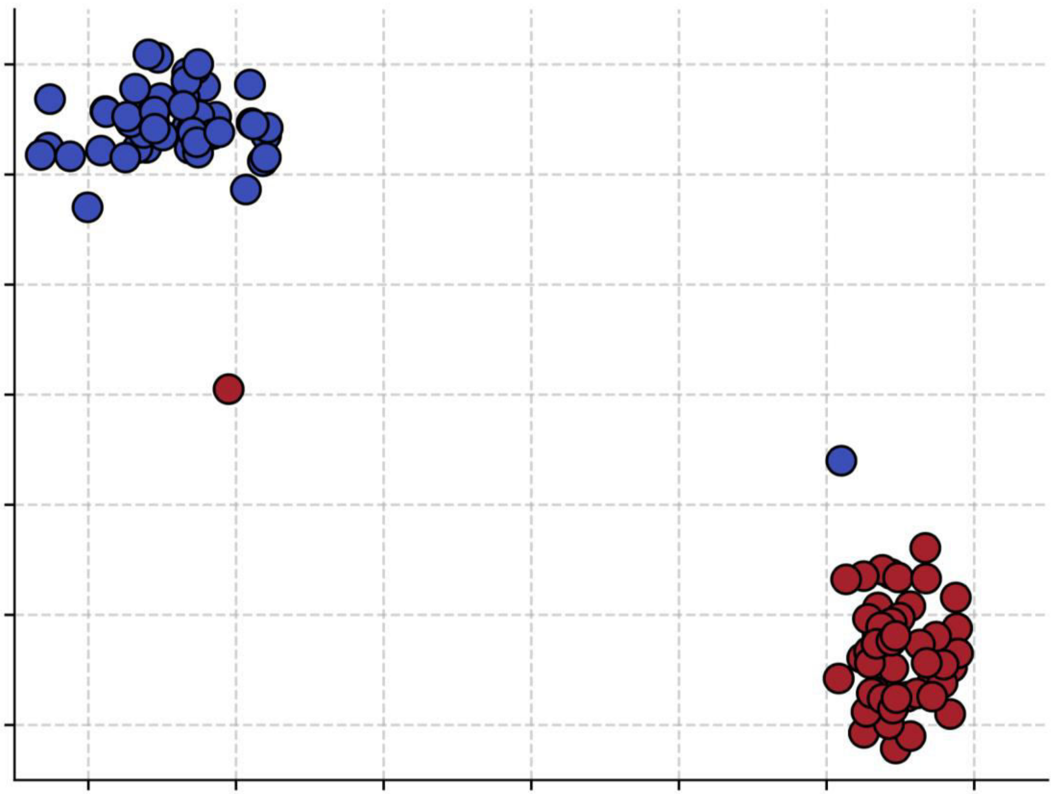
$$min \sum_i \alpha_i - \sum_i \sum_j \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

$$subject\ to\ \alpha_i \geq 0$$

- Primal has as many params as features (n)
- Dual has as many params as samples (l)
- It is more efficient to optimize primal if $l \gg n$

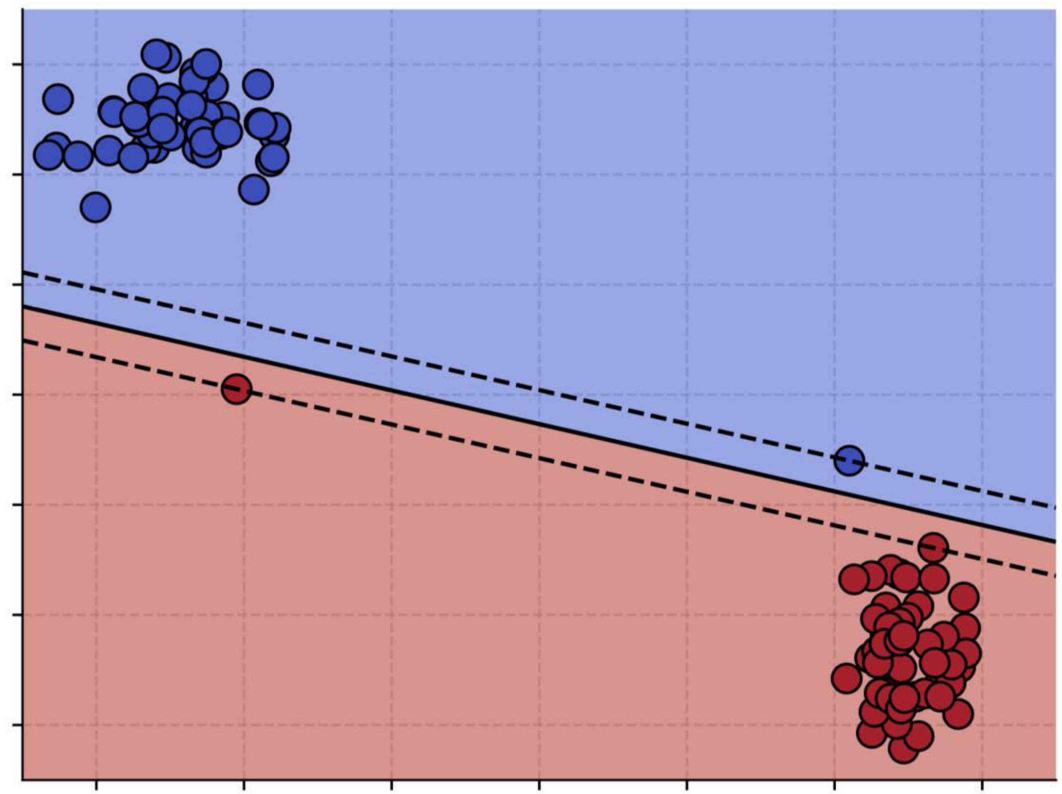
SVM (Soft Margin)

- What happens when we train a hard-margin SVM on this data set?



SVM (Soft Margin)

- What happens when we train a hard-margin SVM on this data set?
- It succeeds at separating the training samples, but with a very tight margin



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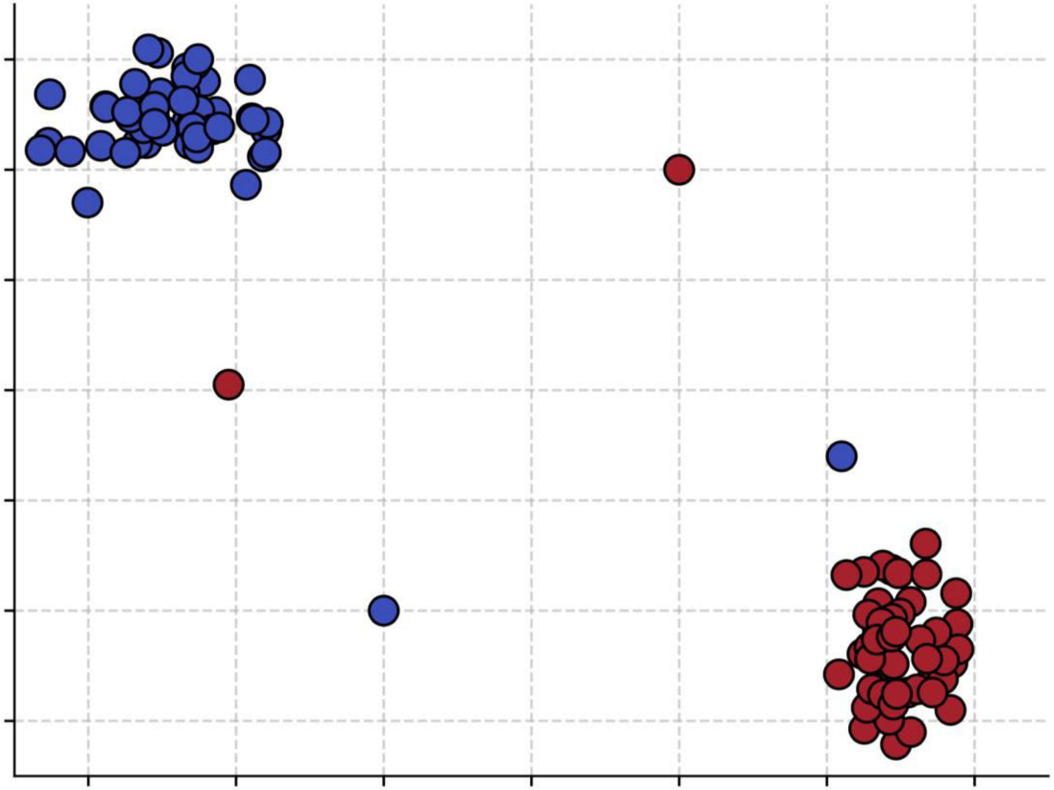
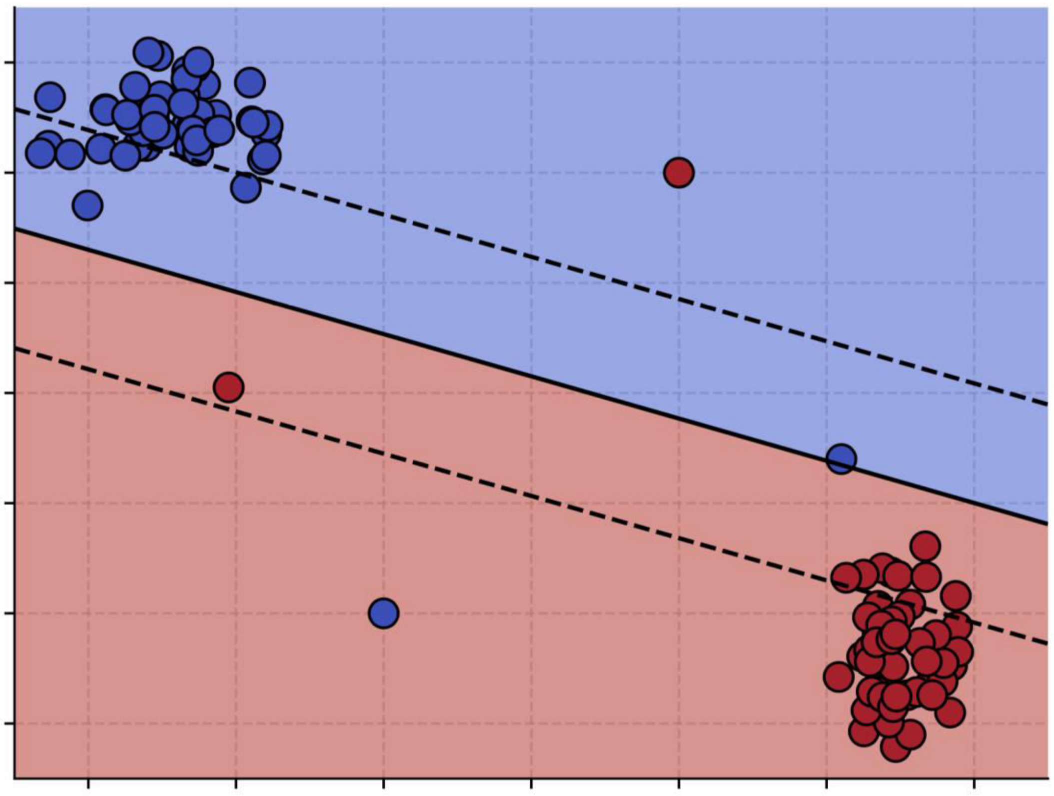


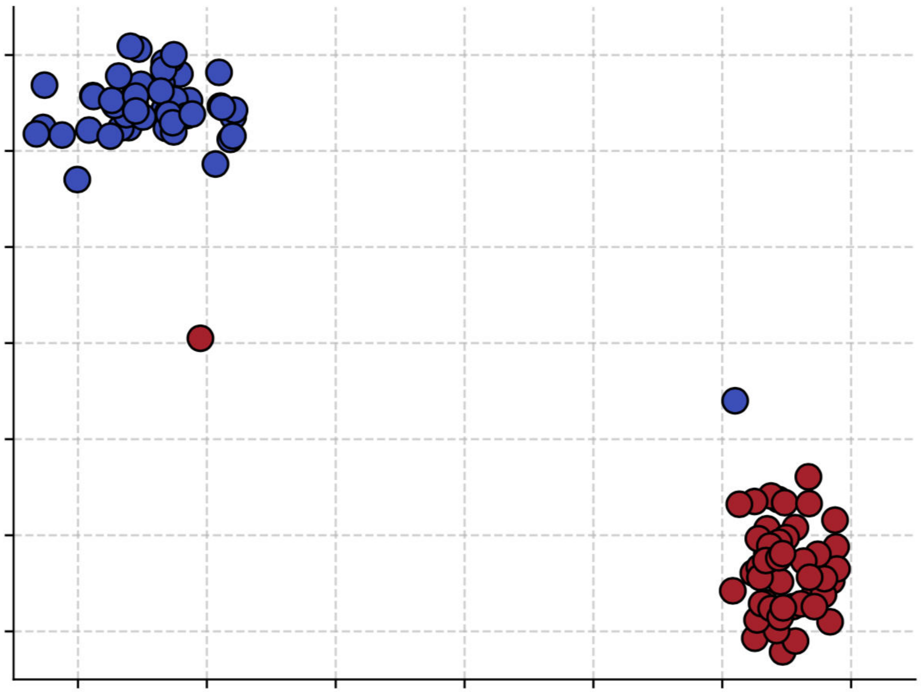
SVM (Soft Margin)

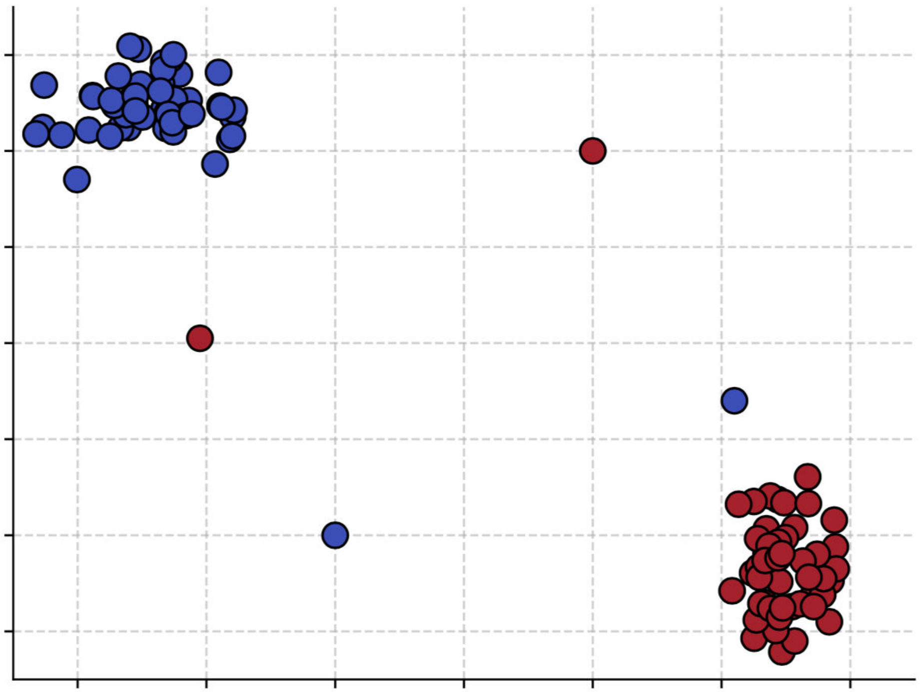
- What happens when we train a hard-margin SVM on this data set?
- It fails, because the samples are not linearly separable



SVM (Soft Margin)

- What would the more “reasonable” solutions be?





SVM (Soft Margin)

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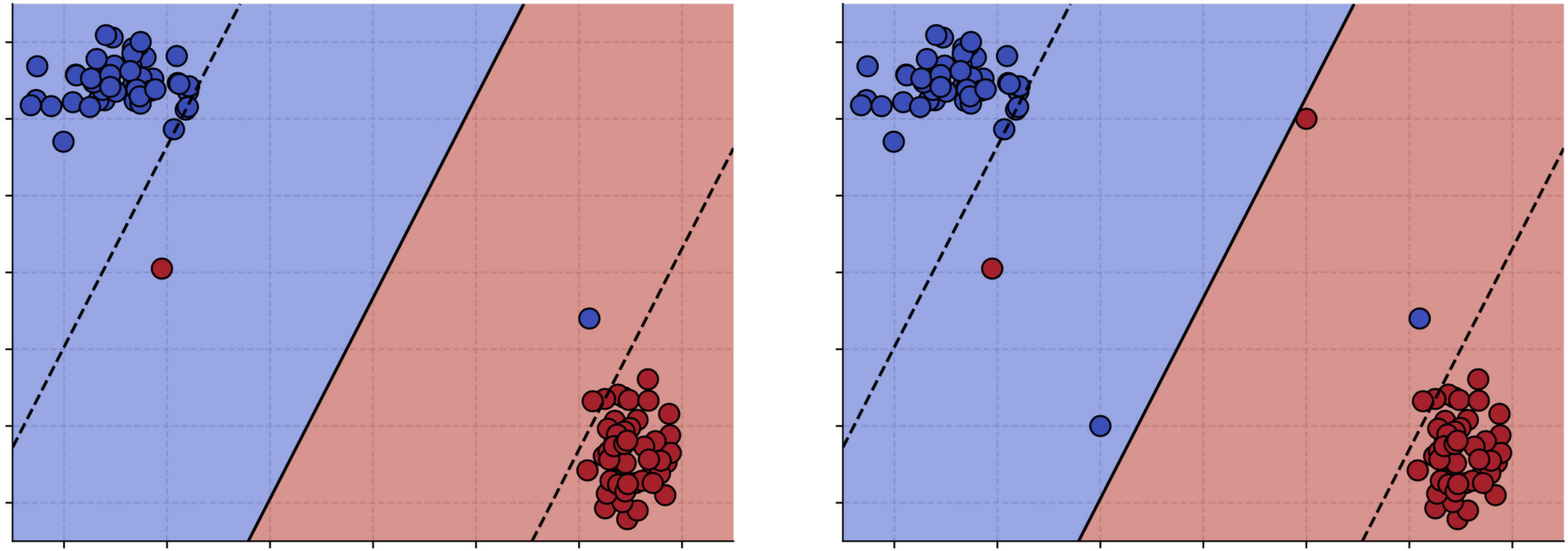
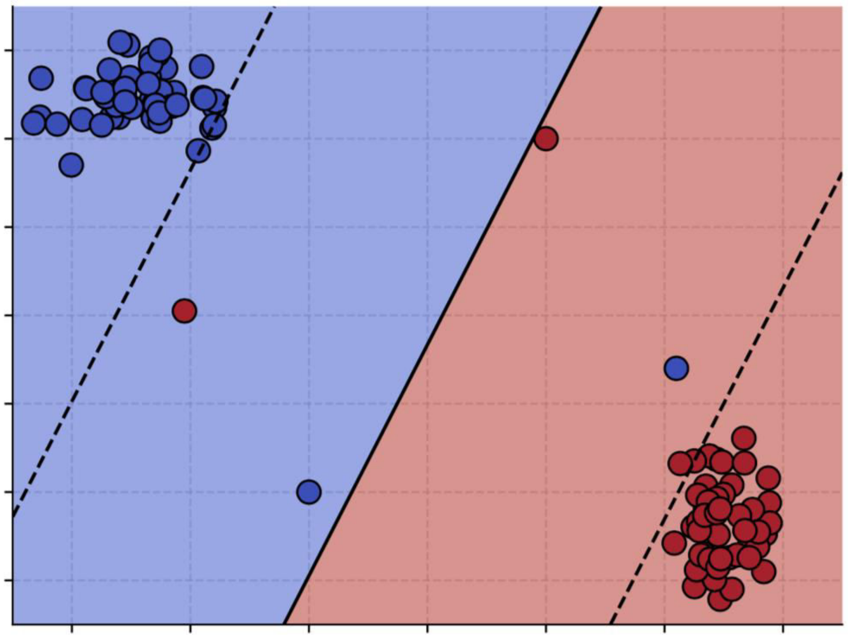


SVM (Soft Margin)

- Allow some training samples to be misclassified, at a cost.

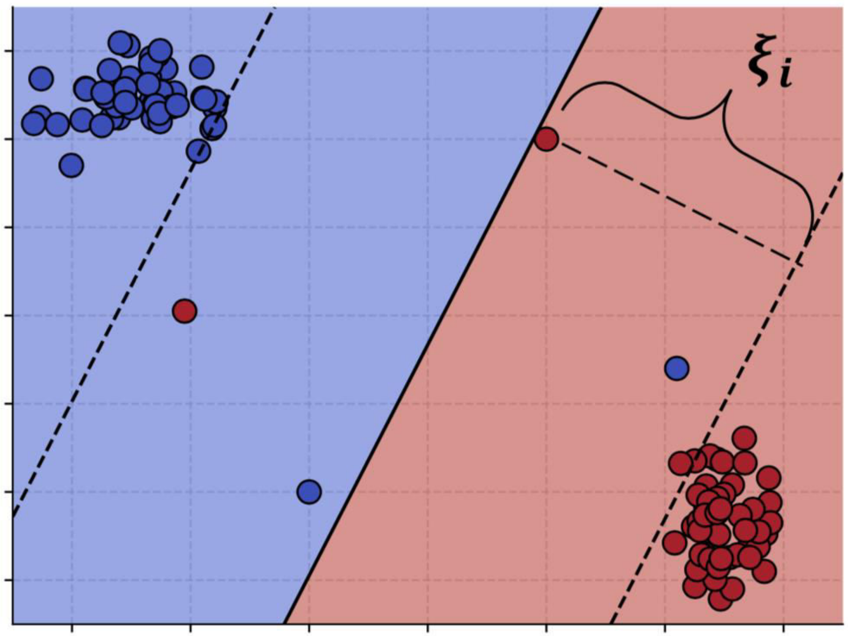


SVM (Soft Margin)

- Allow some training samples to be misclassified, at a cost.
- We introduce slack variables $\xi_i \geq 0$ (how much example x_i is allowed to cross the border):

$$y_i(\langle w, x_i \rangle + b) - 1 \geq 0 \text{ becomes}$$

$$y_i(\langle w, x_i \rangle + b) - 1 \geq -\xi_i$$



- The optimization problem becomes:

$$min\|w\|^2 + C \sum_i \xi_i$$

$$subject\ to\ y_i(\langle w, x_i \rangle + b) - 1 \geq -\xi_i$$

- Trade-off between making the margin wide and allowing training mistakes
- C controls the weight of the mistakes

SVM (Soft Margin)

- When the examples are non-linearly separable:

$$\min_{\mathbf{w},b,\gamma,\xi} -\gamma + C\sum_{i=1}^{\ell}\xi_i$$

subject to

$$y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq \gamma - \xi_i$$

$$\xi_i \geq 0 \quad i = 1, \ldots, \ell$$

$$\|\mathbf{w}\|^2 = 1$$

$$\Longleftrightarrow$$

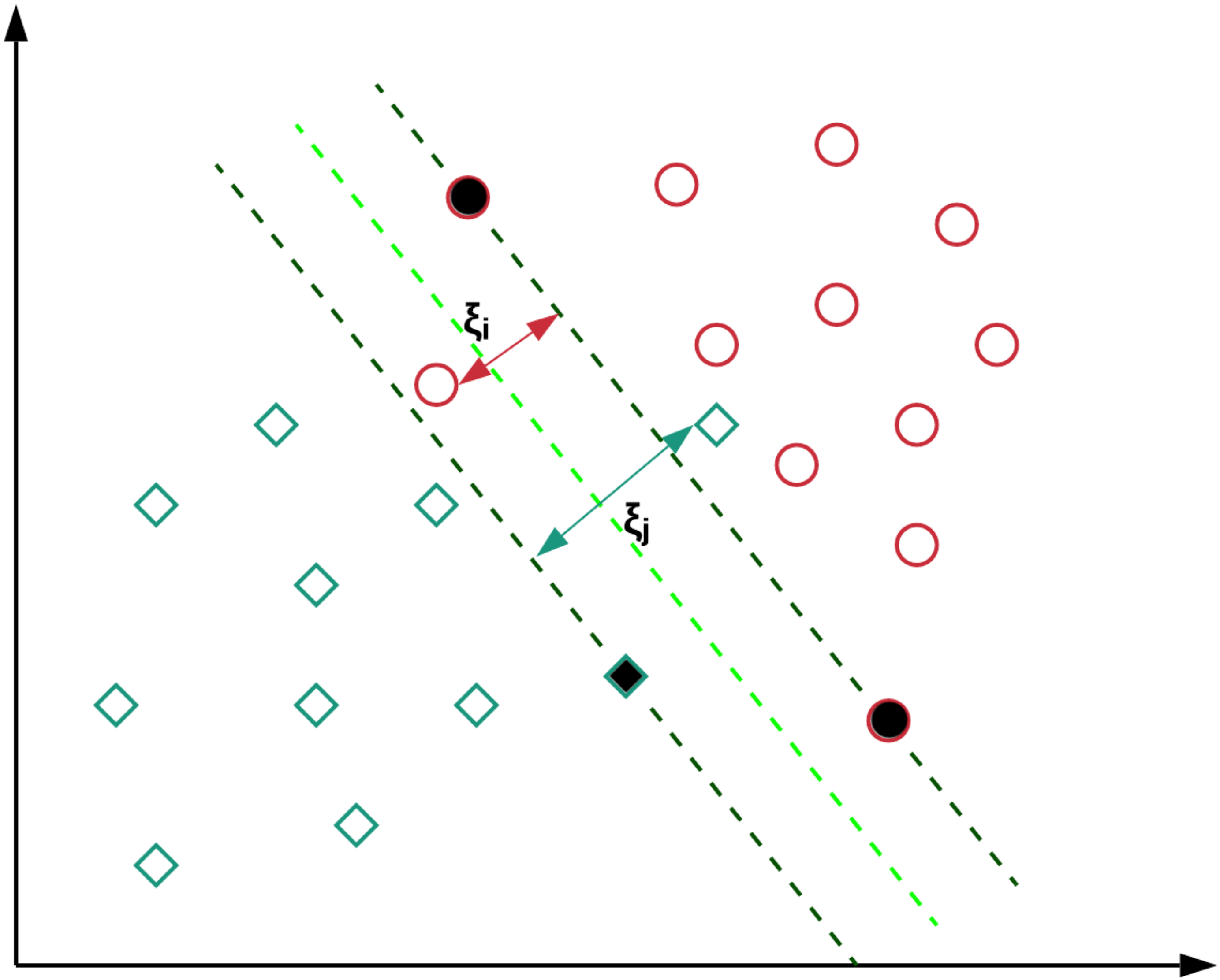
$$\min_{\mathbf{w},b,\xi} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{\ell}\xi_i$$

subject to

$$y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0 \quad i = 1, \ldots, \ell$$

SVM (Soft Margin)



Hinge Loss

$$\left.\begin{aligned} & min\|w\|^2 + C\sum_i \xi_i \\ & subject\ to\ y_i(\langle w, x_i\rangle + b) - 1 \geq -\xi_i \\ & \qquad\qquad \xi_i \geq 0 \end{aligned}\right\} \xi_i = \max\big(0, 1 - y_i(\langle w, x_i\rangle + b)\big)$$

- By replacing ξ_i in the minimization problem, we get:

$$min\|w\|^2 + C\sum_i \max\big(0, 1 - y_i(\langle w, x_i\rangle + b)\big)$$

Hinge Loss

$$min\|w\|^2 + C\sum_i \max\big(0, 1 - y_i(\langle w, x_i\rangle + b)\big)$$

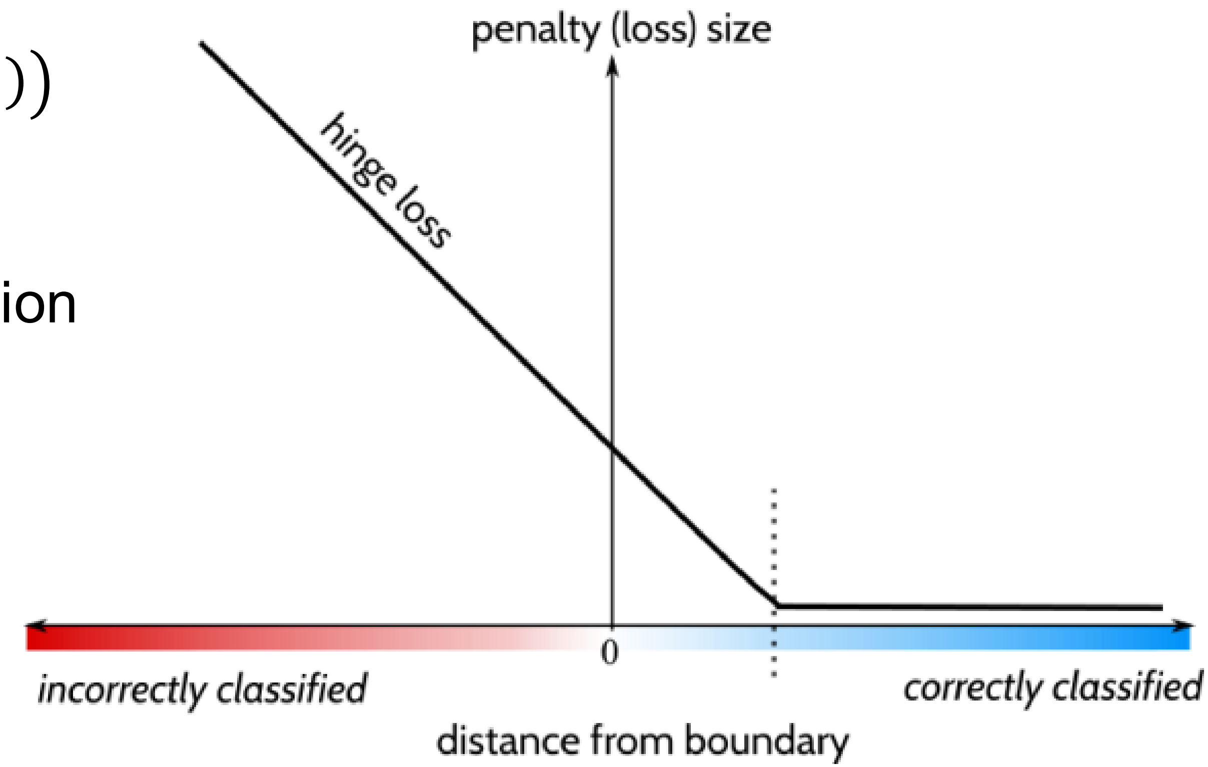
- The hinge loss is defined as follows:

$$\mathrm{L}(x_i) = \max\big(0, 1 - y_i(\langle w, x_i\rangle + b)\big)$$

- We can rewrite the minimization

problem as follows:

$$min\left(C\sum_i \mathrm{L}(x_i) + \|w\|^2\right)$$



- Note: The soft-margin SVM is actually minimizing the hinge loss with regularization

SVM (Soft Margin)

- Allow some training samples to be misclassified, at a cost.
- We introduce slack variables $\xi_i \geq 0$ (how much example x_i is allowed to cross the border):

$$y_i(\langle w, x_i \rangle + b) - 1 \geq 0 \text{ becomes}$$

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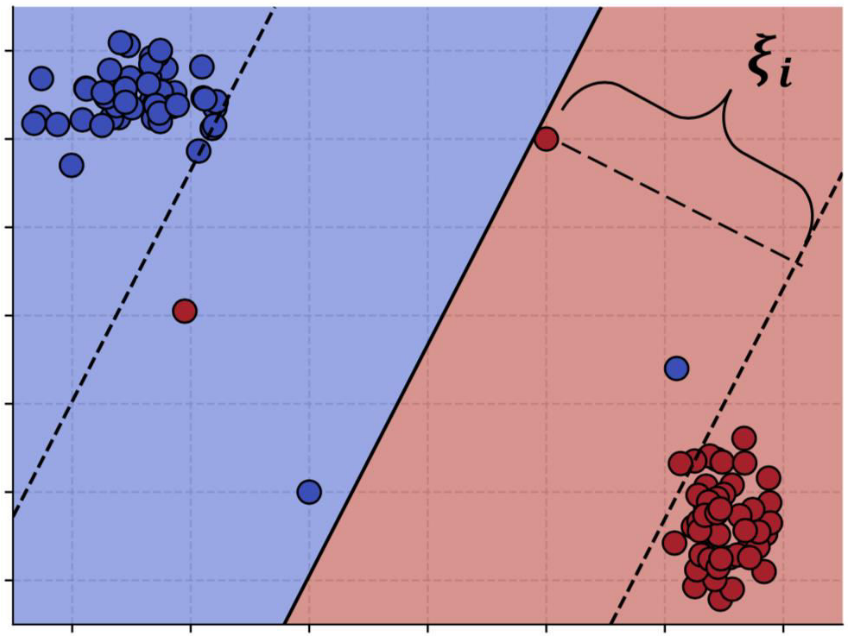


- The optimization problem becomes:

$$min\|w\|^2 + C\sum_i \xi_i$$

$$subject\ to\ y_i(\langle w, x_i \rangle + b) - 1 \geq -\xi_i$$

- Trade-off between making the margin wide and allowing training mistakes
- C controls the weight of the mistakes

SVM (Soft Margin)

- The decision rule (in primal form) is:

$$x \text{ is positive if } \langle w, x \rangle + b \geq 0$$

- In order to obtain w and b, we have to:

$$min\|w\|^2 + C\sum_i \xi_i$$

$$subject\ to\ y_i(\langle w, x_i \rangle + b) - 1 \geq -\xi_i$$

Or

$$min\|w\|^2 + C\sum_i \max\big(0, 1 - y_i(\langle w, x_i \rangle + b)\big)$$

SVM Dual (Soft Margin)

- The decision rule (in dual form) is:

  x is positive if $\sum_i \alpha_i y_i \langle x_i, x \rangle + b \geq 0$

- In order to obtain α_i and b, we have to:

$$min \sum_i \alpha_i - \sum_i \sum_j \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

$$subject\ to\ 0 \leq \alpha_i \leq C, \forall i$$

- Note: we add an upper bound on the Lagrange multipliers

SVM (Python)

- Scikit-learn:

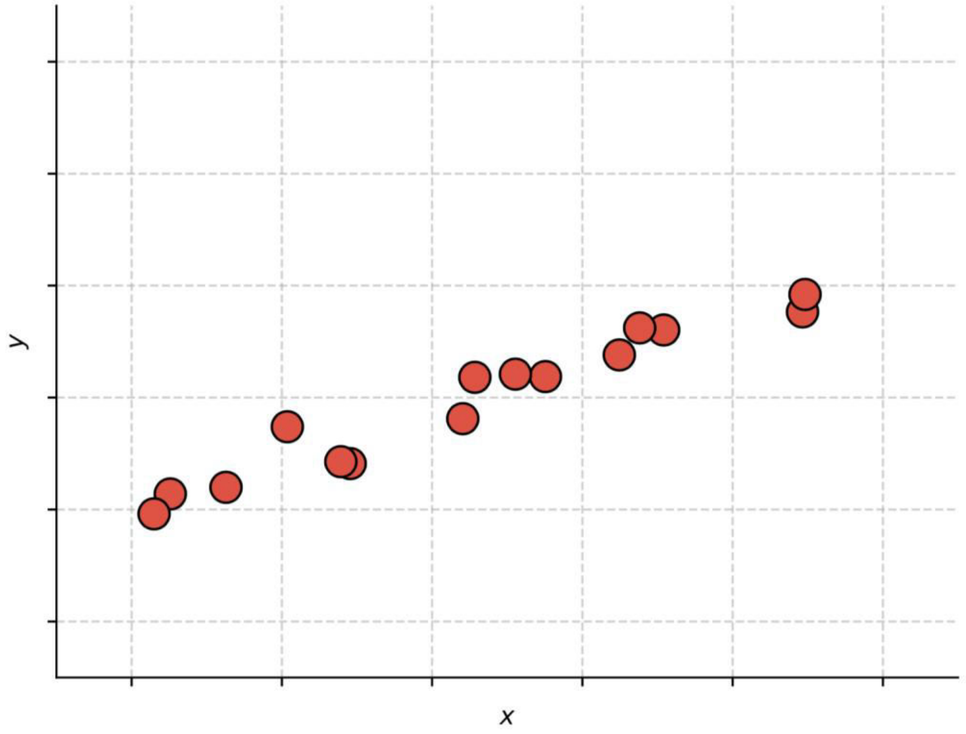
https://scikit-learn.org/stable/modules/svm.html#svm-classification

```
from sklearn import svm

clf = svm.SVC(C = 1.0)

clf.fit(X_train, T_train)

Y_test = clf.predict(X_test)
```

- Plus many other classifiers (based on same use pattern)

Support Vector Regression

- Training: find the flattest function that can fit the training data inside a tube of radius ϵ
- Inference: prediction is based on: $\hat{y} = \langle w, x \rangle + b$



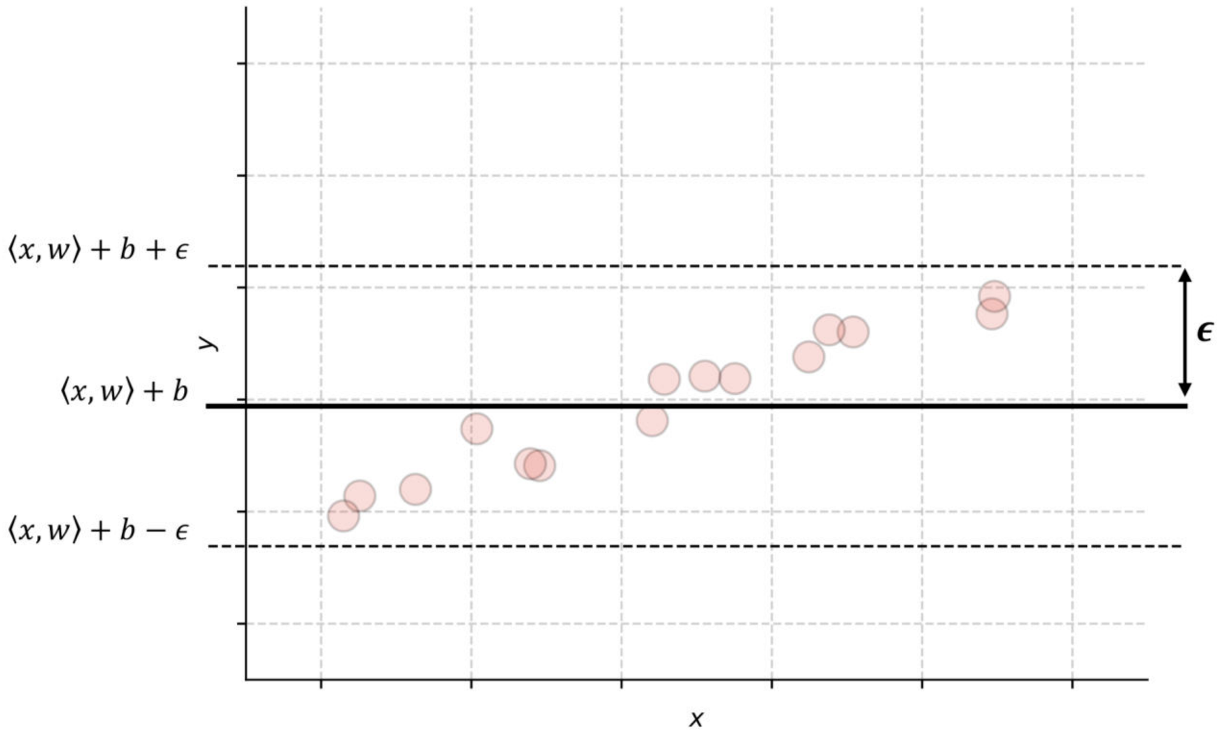
Support Vector Regression

- Training: find the flattest function that can fit the training data inside a tube of radius ϵ
- Inference: prediction is based on: $\hat{y} = \langle w, x \rangle + b$

- Flat function = does not change much with parameters, i.e. small $\|w\|$
- We need to find the smallest $\|w\|$ for which the prediction error is at most ϵ:

$$min\|w\|^2$$

$$subject\ to\ |y_i - (\langle w, x_i \rangle + b)| \leq \epsilon$$



Extreme case: we can fit all data points with a function that does not change at all, i.e. $\|w\| = 0$.

Support Vector Regression

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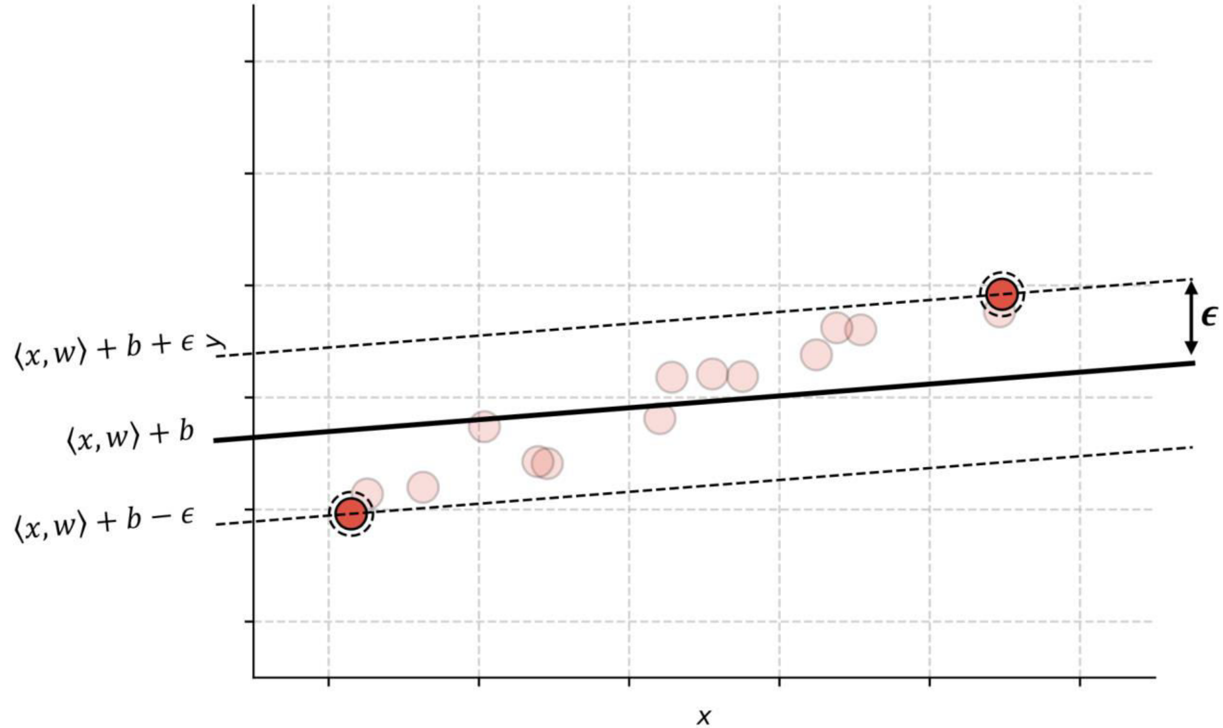

When ϵ is small, w and b need to be adjusted in order to fit all data points.

Support Vector Regression

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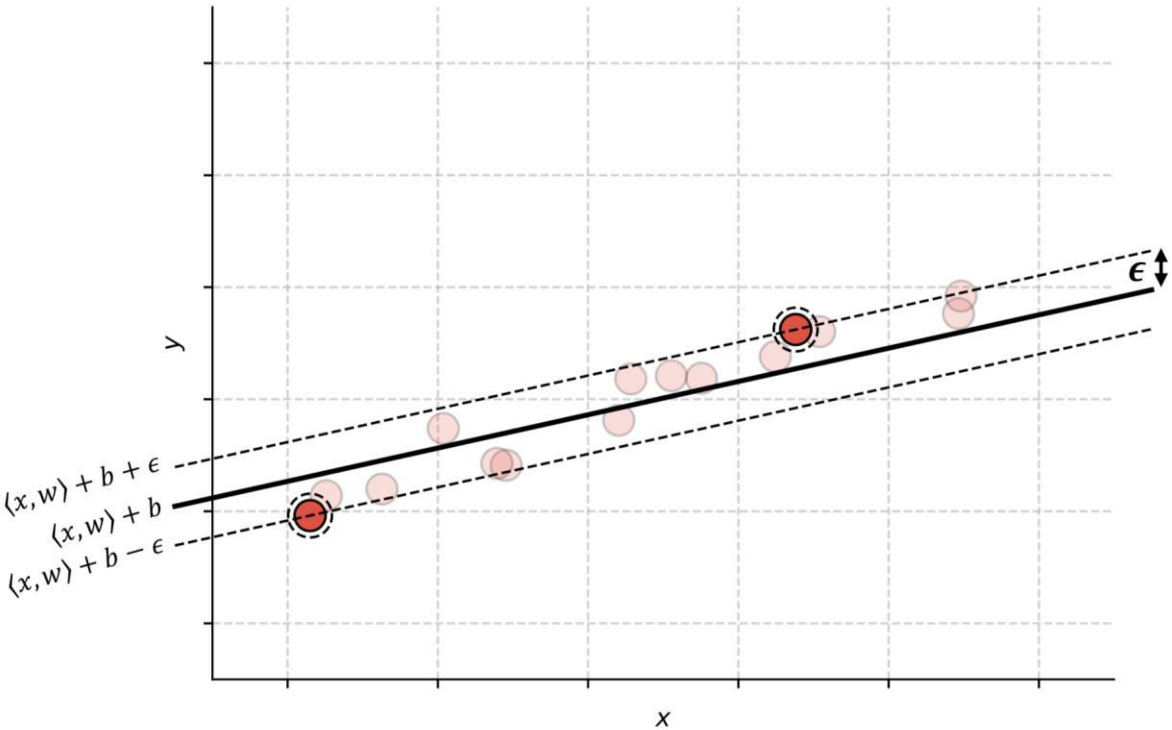

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Support Vector Regression

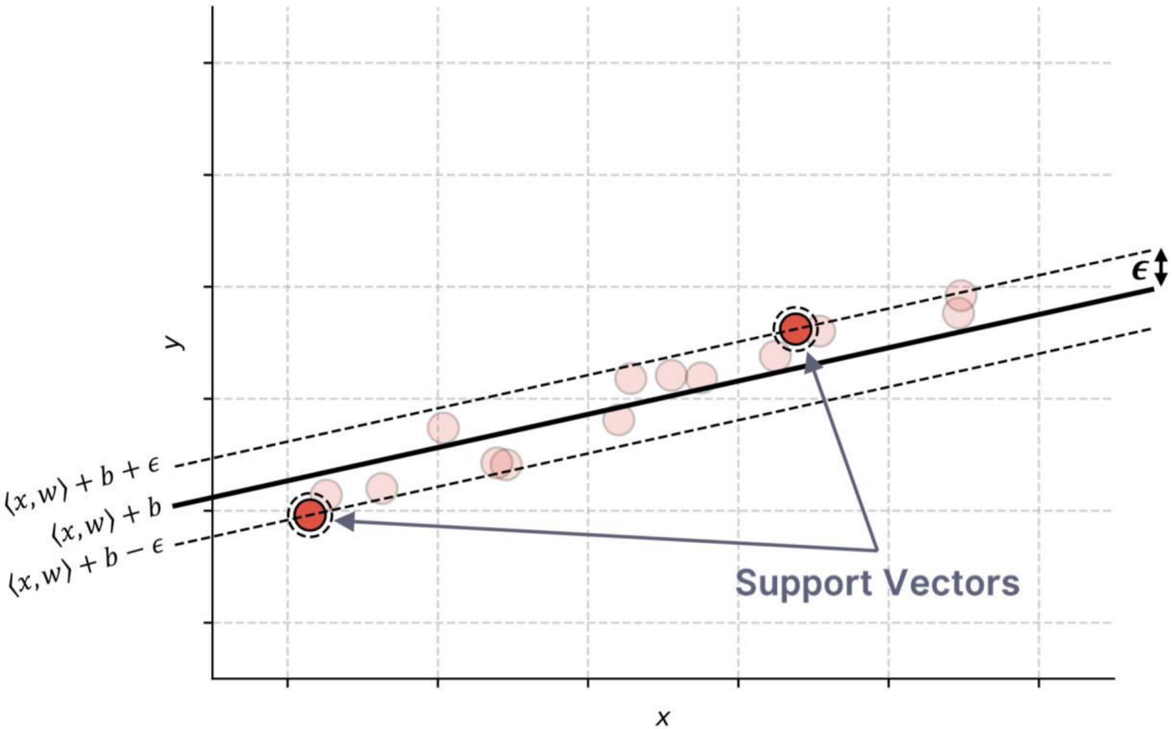
- Training: find the flattest function that can fit the training data inside a tube of radius ϵ
- Inference: prediction is based on: $\hat{y} = \langle w, x \rangle + b$

- Flat function = does not change much with parameters, i.e. small $||w||$
- We need to find the smallest $||w||$ for which the prediction error is at most ϵ:

$$min||w||^2$$

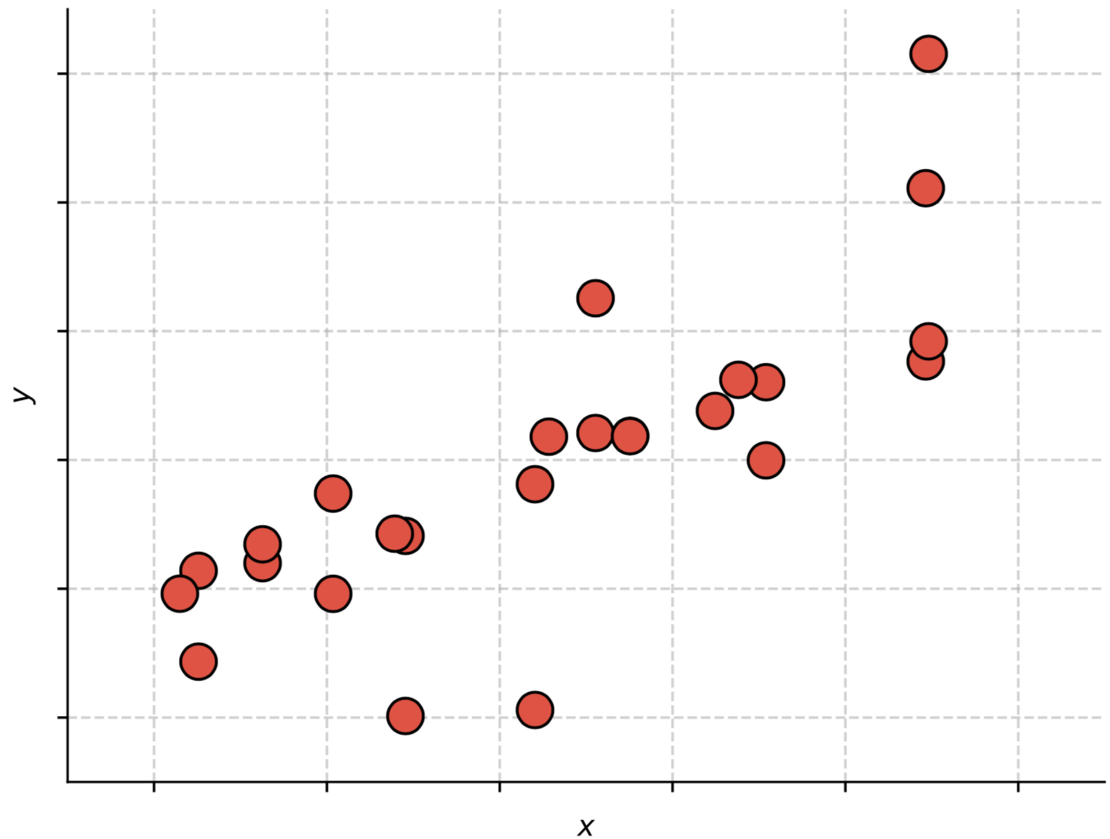
$$subject\ to\ |y_i - (\langle w, x_i \rangle + b)| \leq \epsilon$$

- The model can be expressed only in terms of the scalar product of some training samples (support vectors), i.e. we can apply kernel functions



SVR (Soft Margin)

- Training: find the flattest function that can fit the training data inside a tube of radius ϵ
- Inference: prediction is based on: $\hat{y} = \langle w, x \rangle + b$
- Sometimes it is not reasonable to find a function that fits all training samples inside a tube of radius ϵ



SVR (Soft Margin)

- Training: find the flattest function that can fit the training data inside a tube of radius ϵ
- Inference: prediction is based on: $\hat{y} = \langle w, x \rangle + b$

- Sometimes it is not reasonable to find a function that fits all training samples inside a tube of radius ϵ
- We introduce slack variables:

$$min\|w\|^2 + C\sum_i \xi_i$$

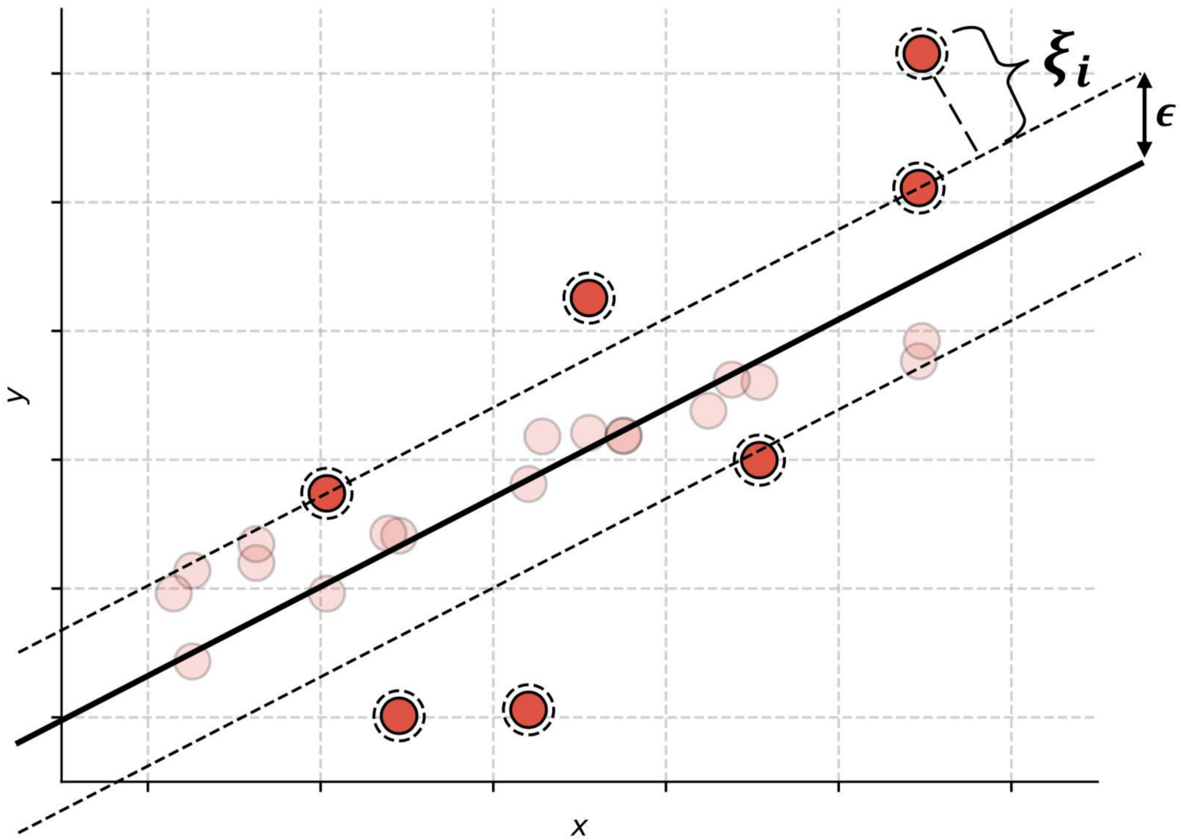
$$subject\ to\ |y_i - (\langle w, x_i \rangle + b)| \leq \epsilon + \xi_i$$

- We define the ϵ-insensitive loss:

$$\mathrm{L}(x_i) = \max(0, |y_i - (\langle w, x_i \rangle + b)| - \epsilon)$$

- And the optimization becomes:

$$min\left(C\sum_i \mathrm{L}(x_i) + \|w\|^2\right)$$

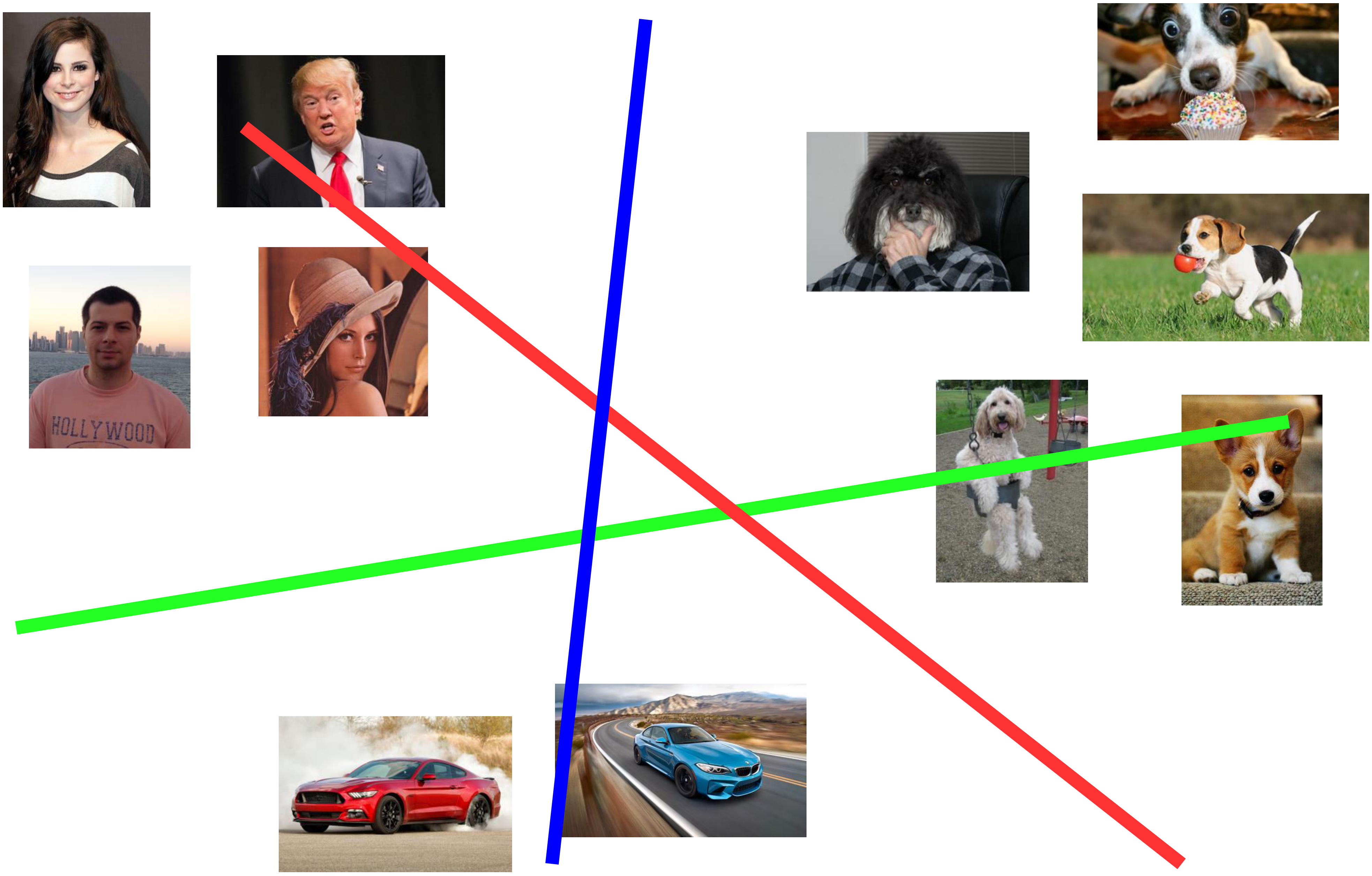


How do we solve many class problems?

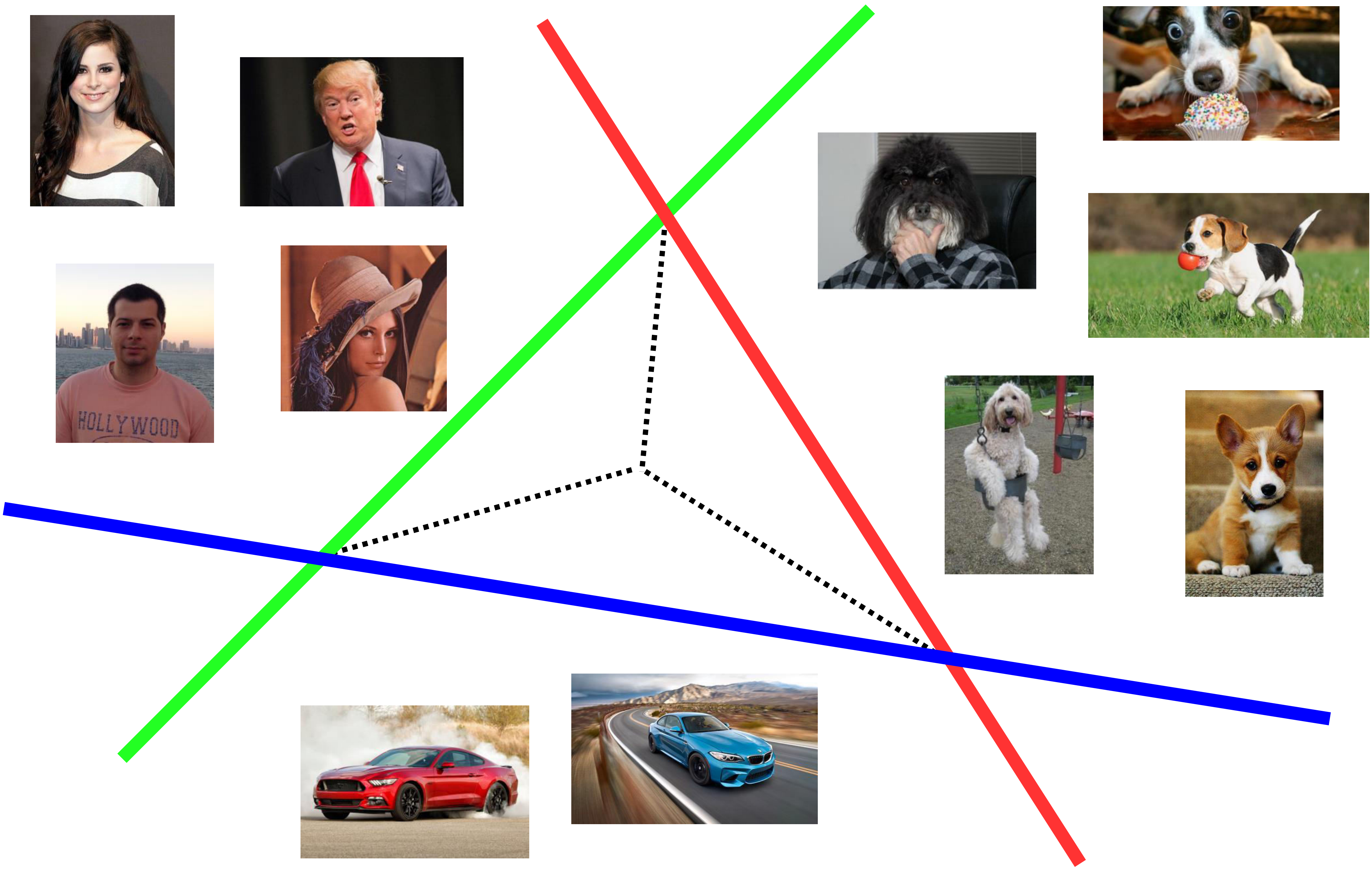
- Schemes for combining multiple binary classifiers:

1) One-versus-one
2) One-versus-all

One-versus-one



One-versus-all



How do we solve many class problems?

- Using classification methods able to handle the multi-class problem directly:

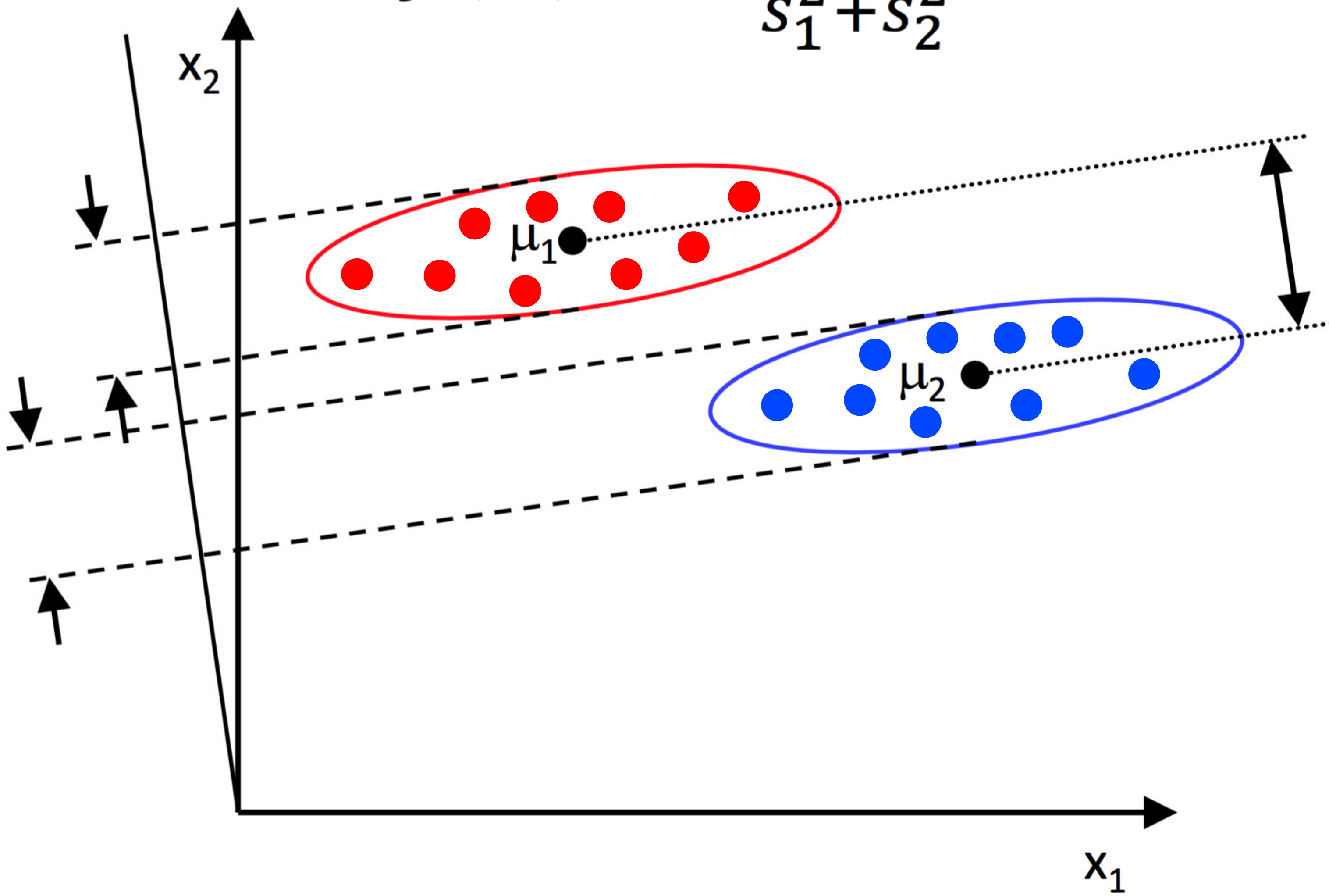
1) Linear (Fisher) Discriminant Analysis
2) Neural Networks (Lectures 7, 8, 9)
3) Random forests (Lecture 5)

Linear Discriminant Analysis

- Each class is approximated with a multinomial Gaussian distribution
- The optimization algoritm is based on finding a hyperplane to project the data points such that:
  - The distance among class means is maximized
  - The variance of each class is minimized

Linear Discriminant Analysis

$$J(w) = \frac{|\mu_1 - \mu_2|^2}{s_1^2 + s_2^2}$$



Linear Discriminant Analysis (Python)

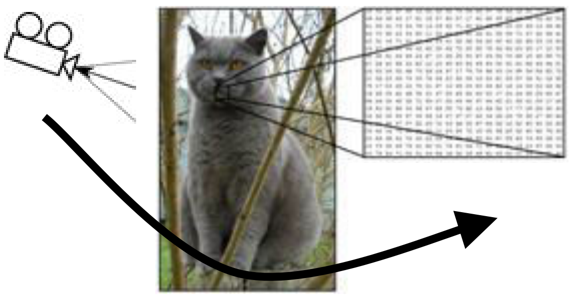
- Scikit-learn:

https://scikit-learn.org/stable/modules/svm.html#svm-classification

```
from sklearn.discriminant_analysis
     import LinearDiscriminantAnalysis
clf = LinearDiscriminantAnalysis()
clf.fit(X_train, T_train)
Y_test = clf.predict(X_test)
```

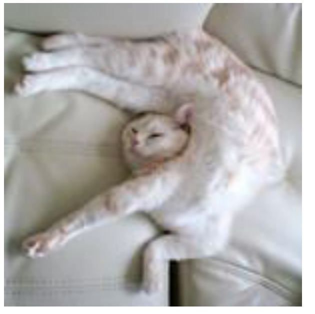
Intra-class variation

Camera angle

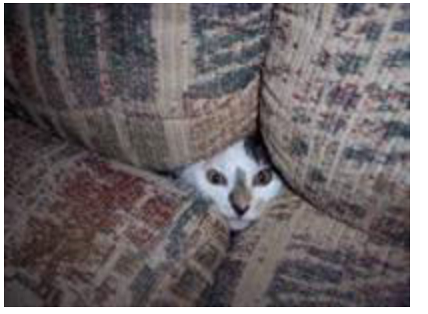


Illumination

Deformation



Occlusion



Confusing background

Intra-class variation

Inter-class similarity

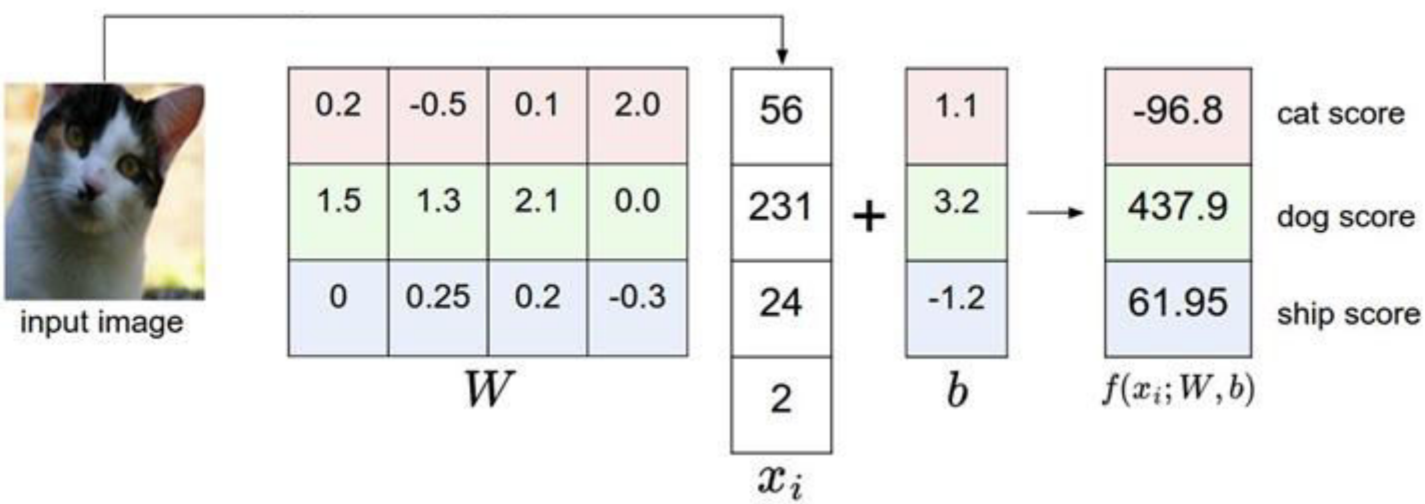
Linear classifier for the multi-class problem

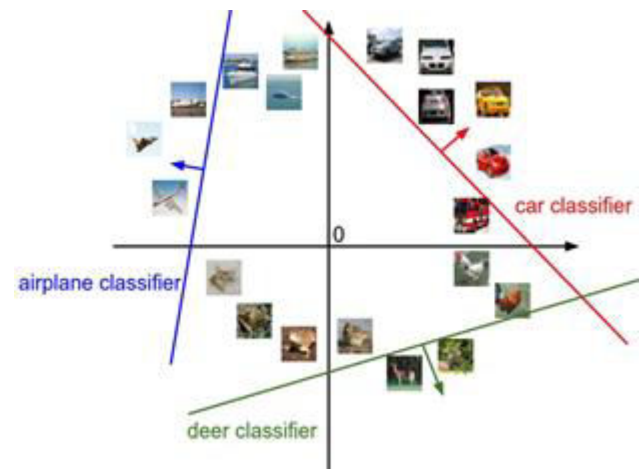
features parameters

$$f(\mathbf{x}, \mathbf{W})$$

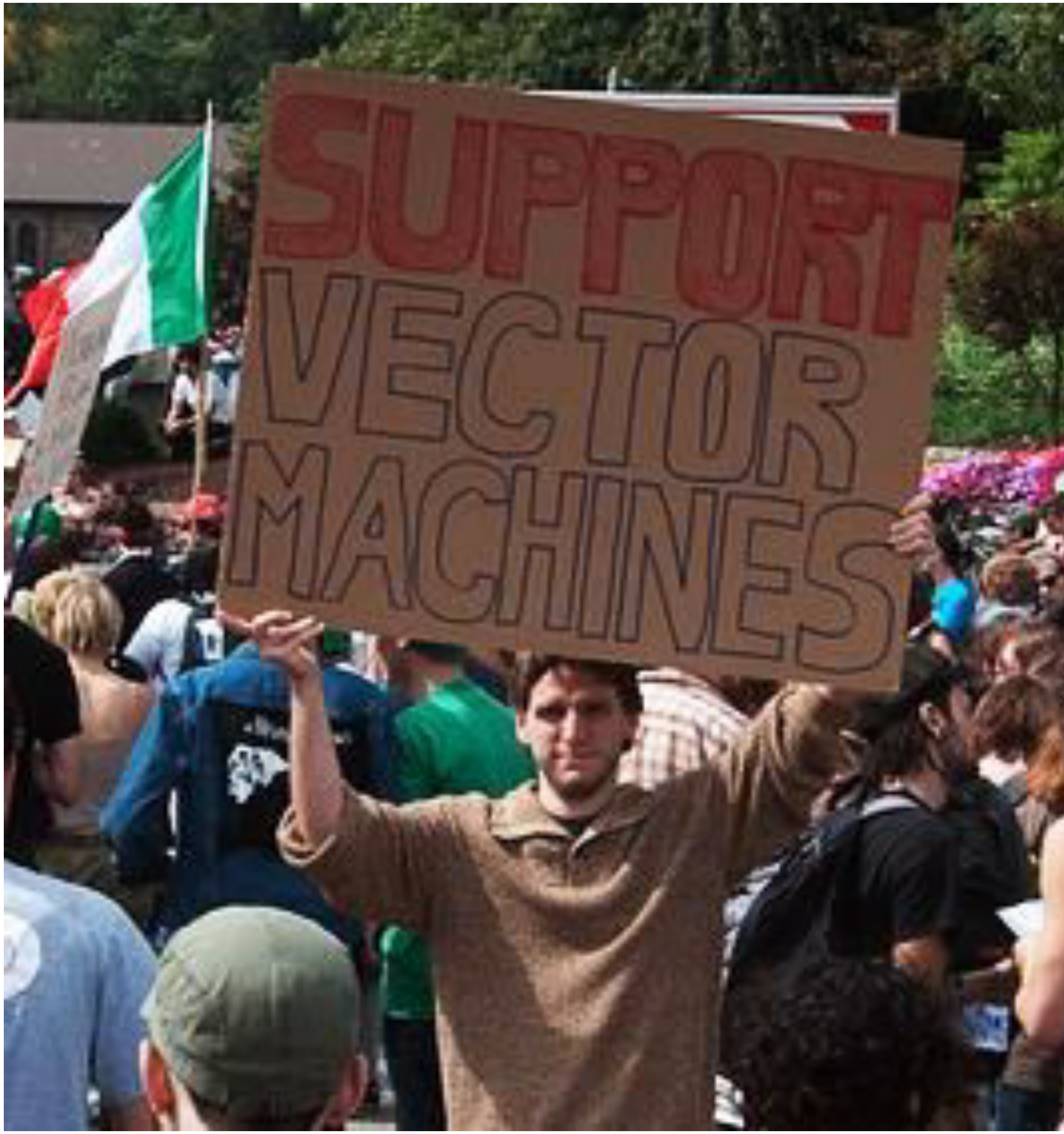
N values that indicate the scores for each class

Feature vector





Linear classifier for the multi-class problem



Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**

Multiclass SVM loss:

Given an example (x_i, y_i), where x_i is the image and where y_i is the (integer) label,

and using the shorthand for the scores vector:

$$s = f(x_i, W)$$

the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

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cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9		

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$$\begin{aligned} &= \max(0, 5.1 - 3.2 + 1) \\ &\quad + \max(0, -1.7 - 3.2 + 1) \\ &= \max(0, 2.9) + \max(0, -3.9) \\ &= 2.9 + 0 \\ &= 2.9 \end{aligned}$$

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



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the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

$= \max(0, 1.3 - 4.9 + 1)$
$+\max(0, 2.0 - 4.9 + 1)$
$= \max(0, -2.6) + \max(0, -1.9)$
$= 0 + 0$
$= 0$

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:

  

cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	10.9

Multiclass SVM loss:

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and using the shorthand for the scores vector:

$$s = f(x_i, W)$$

the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

= max(0, 2.2 - (-3.1) + 1)
+max(0, 2.5 - (-3.1) + 1)
= max(0, 5.3) + max(0, 5.6)
= 5.3 + 5.6
= 10.9

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:

cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	10.9

Multiclass SVM loss:

Given an example (x_i, y_i), where x_i is the image and where y_i is the (integer) label,

and using the shorthand for the scores vector:

$$s = f(x_i, W)$$

the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

L = (2.9 + 0 + 10.9)/3
= **4.6**

Softmax (Multinomial Logistic Regression)

scores = unnormalized log probabilities of the classes

$$P(Y=k|X=x_i) = \boxed{\frac{e^{s_k}}{\sum_j e^{s_j}}} \quad \text{where} \quad s = f(x_i; W)$$

Softmax function

cat	**3.2**
car	5.1
frog	-1.7

Want to maximize the log likelihood, or (for a loss function) to minimize the negative log likelihood of the correct class:

$$L_i = -\log P(Y = y_i | X = x_i)$$

In summary: $L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$

Softmax (Multinomial Logistic Regression)

$$L_i = -\log(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}})$$

Q: What is the min/max possible loss L_i?

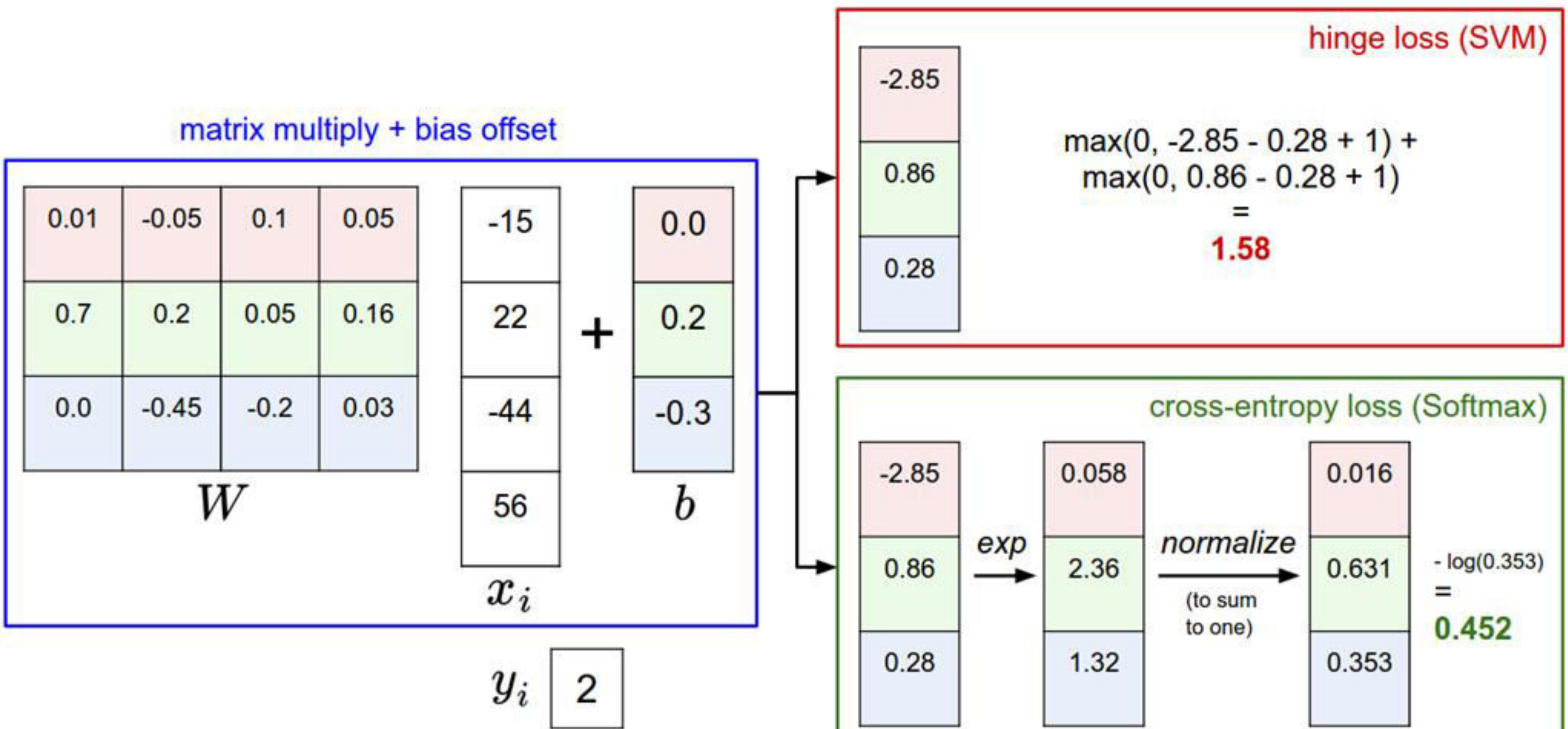
unnormalized probabilities

	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ $L_i = -\log(0.13)$ = **0.89**

unnormalized log probabilities

probabilities



matrix multiply + bias offset
0.01
-0.05
0.1
0.05
0.7
0.2
0.05
0.16
0.0
-0.45
-0.2
0.03
W
-15
22
-44
56
x_i
+
0.0
0.2
-0.3
b
y_i
2
hinge loss (SVM)
-2.85
0.86
0.28
max(0, -2.85 - 0.28 + 1) +
max(0, 0.86 - 0.28 + 1)
=
1.58
cross-entropy loss (Softmax)
-2.85
0.86
0.28
exp
0.058
2.36
1.32
normalize
(to sum
to one)
0.016
0.631
0.353
- log(0.353)
=
0.452

Softmax vs. SVM

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Assume scores:
[10, -2, 3]
[10, 9, 9]
[10, -100, -100]
and $\boxed{y_i = 0}$

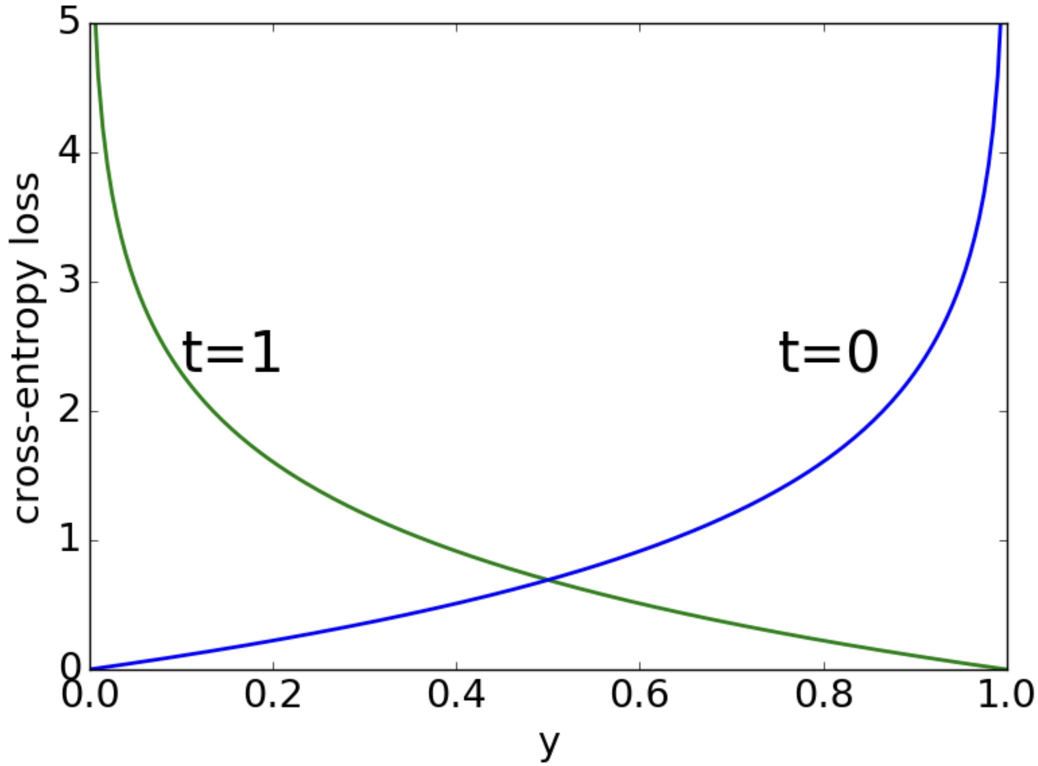
Q: Suppose we take a datapoint and we add some small perturbations (changing its score slightly). What happens to the loss in both cases?

Binary cross-entropy loss

- Binary cross-entropy (logistic) loss:

$$L_i = -(t_i \cdot log(y_i) + (1 - t_i) \cdot log(1 - y_i))$$

where t_i is the ground-truth binary label (0 or 1) of sample x_i, and y_i is the prediction for the same sample



What is the best classification method?

- **“No free lunch” theorem:**

Any two algorithms are equivalent when their (average) performance is measured on all possible tasks

- It follows that there is no shortcut in choosing the right algorithm for you task
- Usually, you have to try several and see which one works best
- Intuition and experience will be useful

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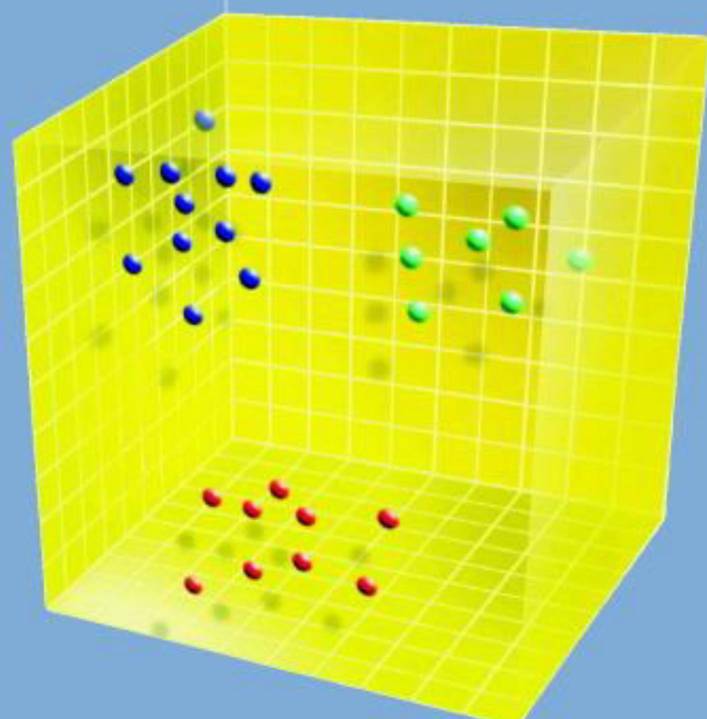

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