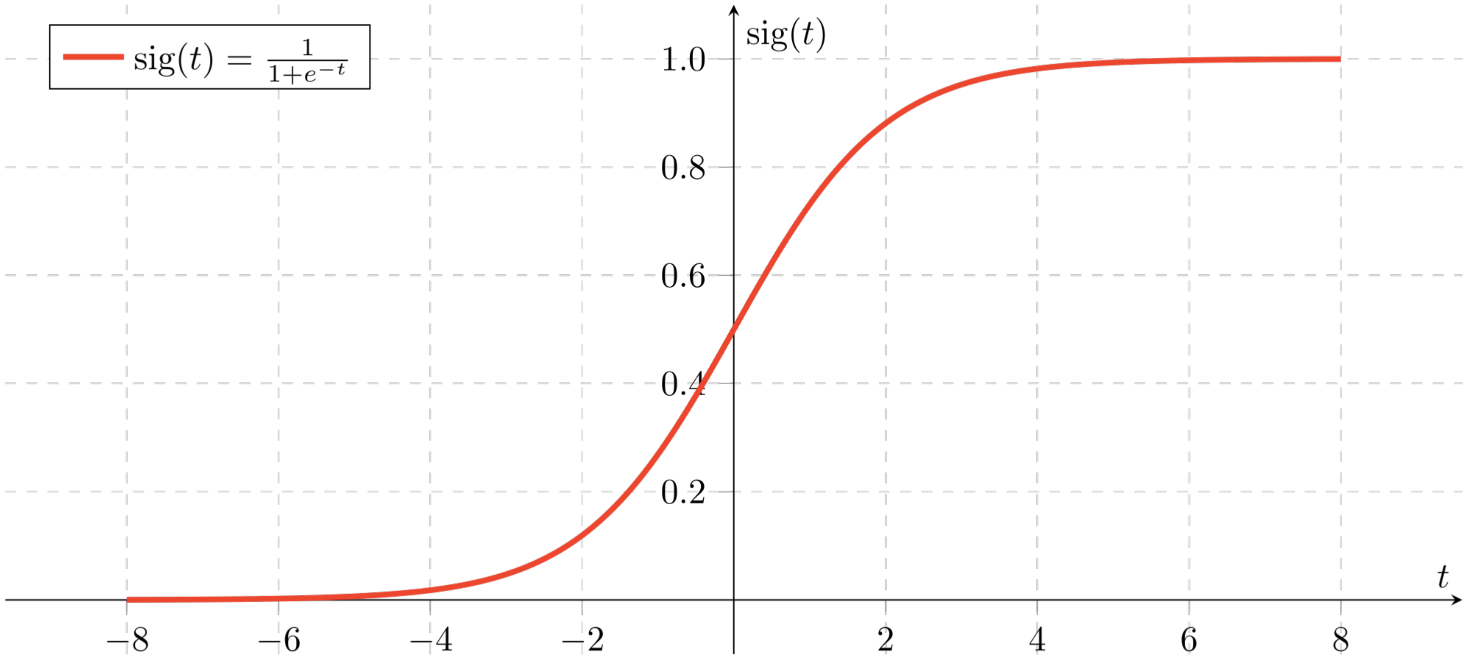
Linear classifiers: Outline

- Examples of classification models: nearest neighbor, linear
- Empirical loss minimization framework
- Linear classification models
  1. Linear regression
  2. Logistic regression
  3. Perceptron training algorithm
  4. Support vector machines
- Multi-class classification

Logistic regression

- Let's learn a probabilistic classifier estimating the probability of the input x having a positive label, given by putting a *sigmoid function* around the linear response $w^T x$:

$$P_w(y = 1|x) = \sigma(w^T x) = \frac{1}{1+\exp(-w^T x)}$$



Logistic loss

- Given: $\{(x_i, y_i), i = 1, \dots, n\}$, $y_i \in \{-1,1\}$
- Maximum (conditional) likelihood estimate: find w that minimizes

$$\hat{L}(w) = -\frac{1}{n}\sum_{i=1}^{n} \log P_w(y_i|x_i)$$

$$l(w, x_i, y_i) = -\log P_w(y_i|x_i)$$

- If $y_i = 1$:

$$P_w(y_i|x_i) = \sigma(w^T x_i)$$

- If $y_i = -1$:

$$P_w(y_i|x_i) = 1 - \sigma(w^T x_i) = \sigma(-w^T x_i)$$

- Thus,

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

Logistic loss

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

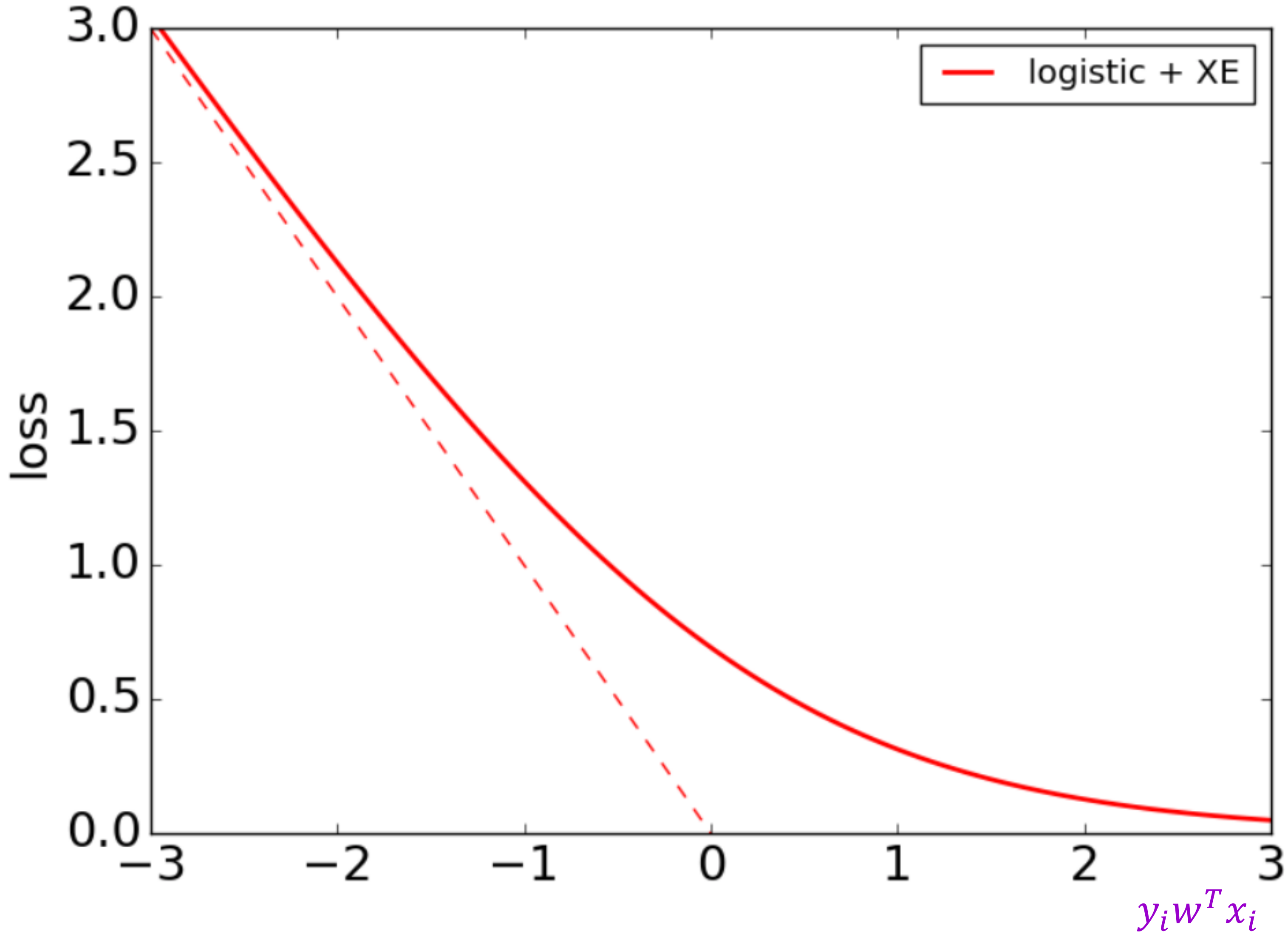


Figure source

Logistic loss: Optimization

- Given: $\{(x_i, y_i), i = 1, \dots, n\}$, $y_i \in \{-1,1\}$
- Find w that minimizes

$$\hat{L}(w) = -\frac{1}{n}\sum_{i=1}^{n} \log P_w(y_i|x_i)$$

$$= -\frac{1}{n}\sum_{i=1}^{n} \log \sigma(y_i w^T x_i)$$

- How do we find the minimum?

Stochastic gradient descent (SGD)

- At each iteration, take a *single data point* (x_i, y_i) and perform a parameter update using $\nabla l(w, x_i, y_i)$, the gradient of the loss for that point:

$$w \leftarrow w - \eta \nabla l(w, x_i, y_i)$$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

- Let's find the gradient:

$$\nabla l(w, x_i, y_i) = -\nabla_w \log \sigma(y_i w^T x_i)$$
$$= -\frac{\nabla_w \sigma(y_i w^T x_i)}{\sigma(y_i w^T x_i)}$$

- Derivative of log:

$$[\log(g(a))]' = \frac{g'(a)}{g(a)}$$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

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$$\nabla l(w, x_i, y_i) = -\nabla_w \log \sigma(y_i w^T x_i)$$

$$= -\frac{\nabla_w \sigma(y_i w^T x_i)}{\sigma(y_i w^T x_i)}$$

$$= -\frac{\sigma(y_i w^T x_i)\sigma(-y_i w^T x_i) y_i x_i}{\sigma(y_i w^T x_i)}$$

Derivative of sigmoid:

$$\sigma'(a) = \sigma(a)(1 - \sigma(a)) = \sigma(a)\sigma(-a)$$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

- Let's find the gradient:

$$\nabla l(w, x_i, y_i) = -\nabla_w \log \sigma(y_i w^T x_i)$$
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$$= -\frac{\sigma(y_i w^T x_i)\sigma(-y_i w^T x_i) y_i x_i}{\sigma(y_i w^T x_i)}$$

- We also used the *chain rule*: $[g_2(g_1(a))]' = g_2'(g_1(a)) g_1'(a)$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

- Let's find the gradient:

$$\nabla l(w, x_i, y_i) = -\nabla_w \log \sigma(y_i w^T x_i)$$
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$$= -\frac{\sigma(y_i w^T x_i)\sigma(-y_i w^T x_i) y_i x_i}{\sigma(y_i w^T x_i)}$$
$$= -\sigma(-y_i w^T x_i) y_i x_i$$

- SGD update:

$$w \leftarrow w + \eta\, \sigma(-y_i w^T x_i) y_i x_i$$

SGD for logistic regression

- Let's take a closer look at the SGD update:

$$w \leftarrow w + \eta\, \sigma(-y_i w^T x_i) y_i x_i$$

- What happens if x_i is *incorrectly,* but confidently, classified?
  - The update rule approaches $w \leftarrow w + \eta\, y_i x_i$
- What happens if x_i is *correctly,* and confidently, classified?
  - The update approaches zero (but never actually reaches zero)
- What happens if all training points are correctly and confidently classified?

SGD for logistic regression

- Logistic regression *does not converge* for linearly separable data!
  - Scaling w by ever larger constants makes the classifier more confident and keeps increasing the likelihood of the data

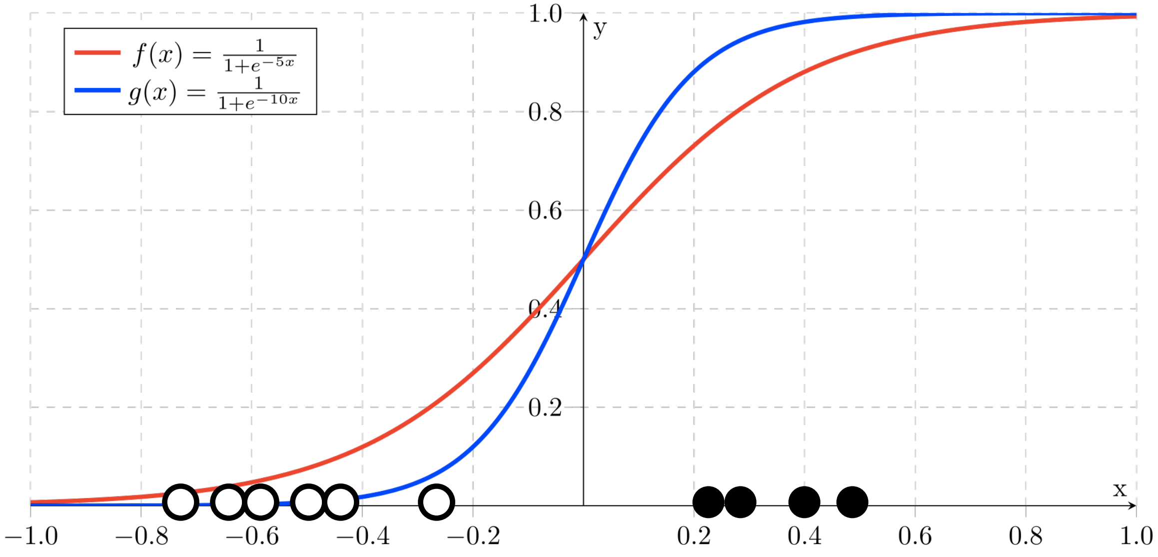

Image source

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Recall: The shape of logistic loss

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

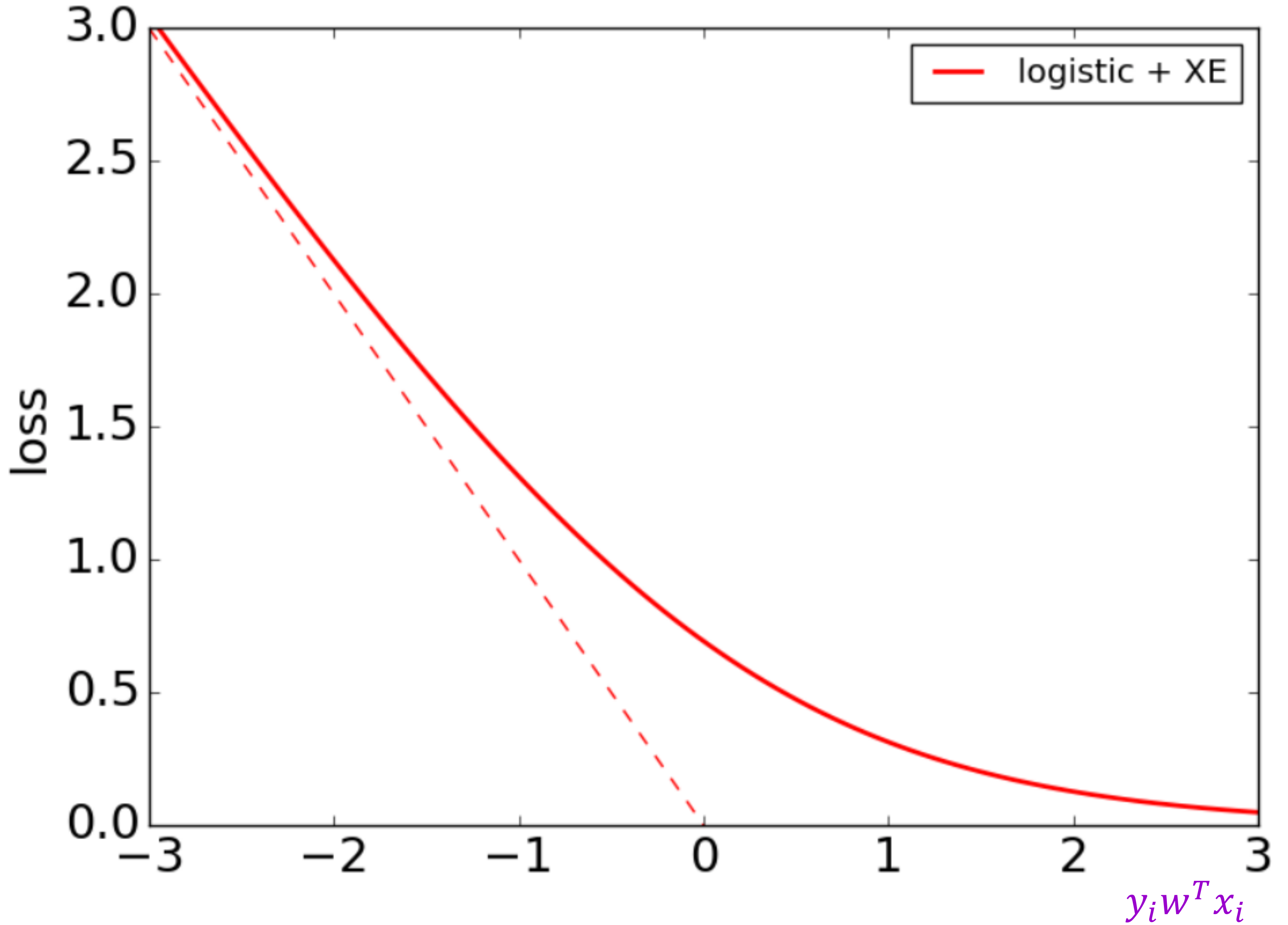
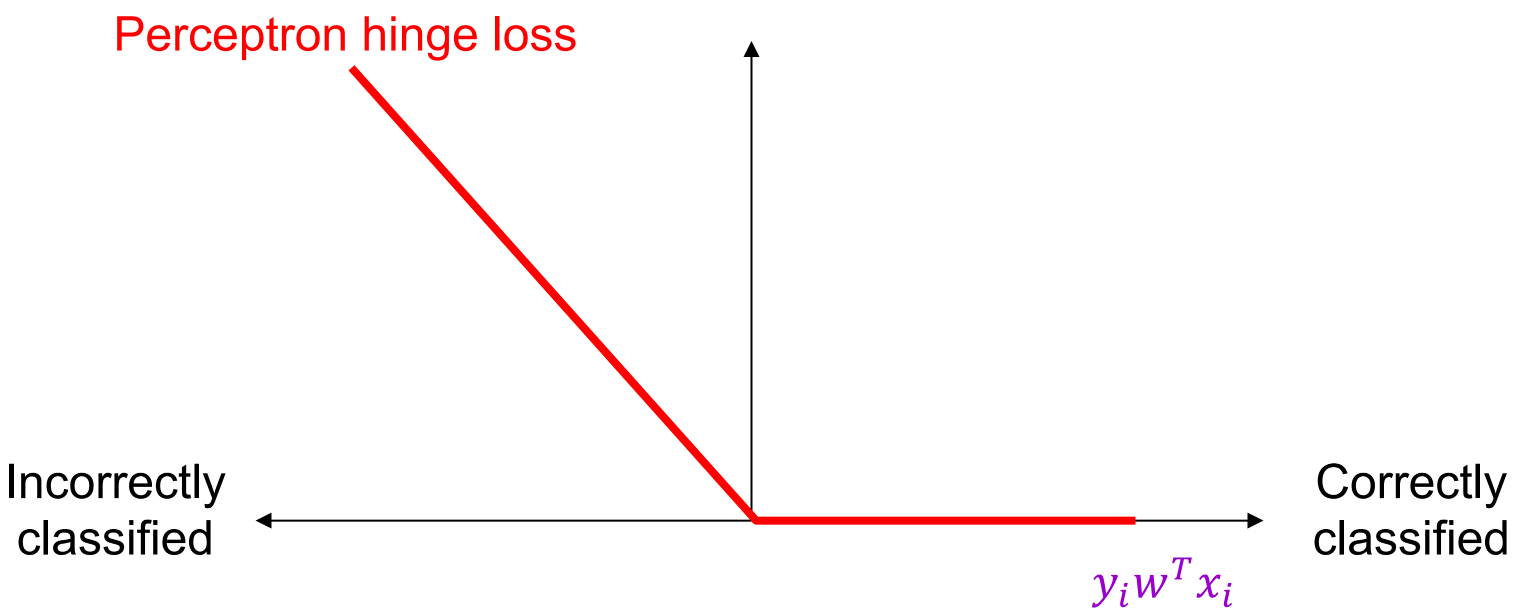


Figure source

Perceptron

- Let's define the *perceptron hinge loss*:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$



Perceptron

- Let's define the *perceptron hinge loss*:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

- Training: find w that minimizes

$$\hat{L}(w) = \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i) = \frac{1}{n}\sum_{i=1}^{n} \max(0, -y_i w^T x_i)$$

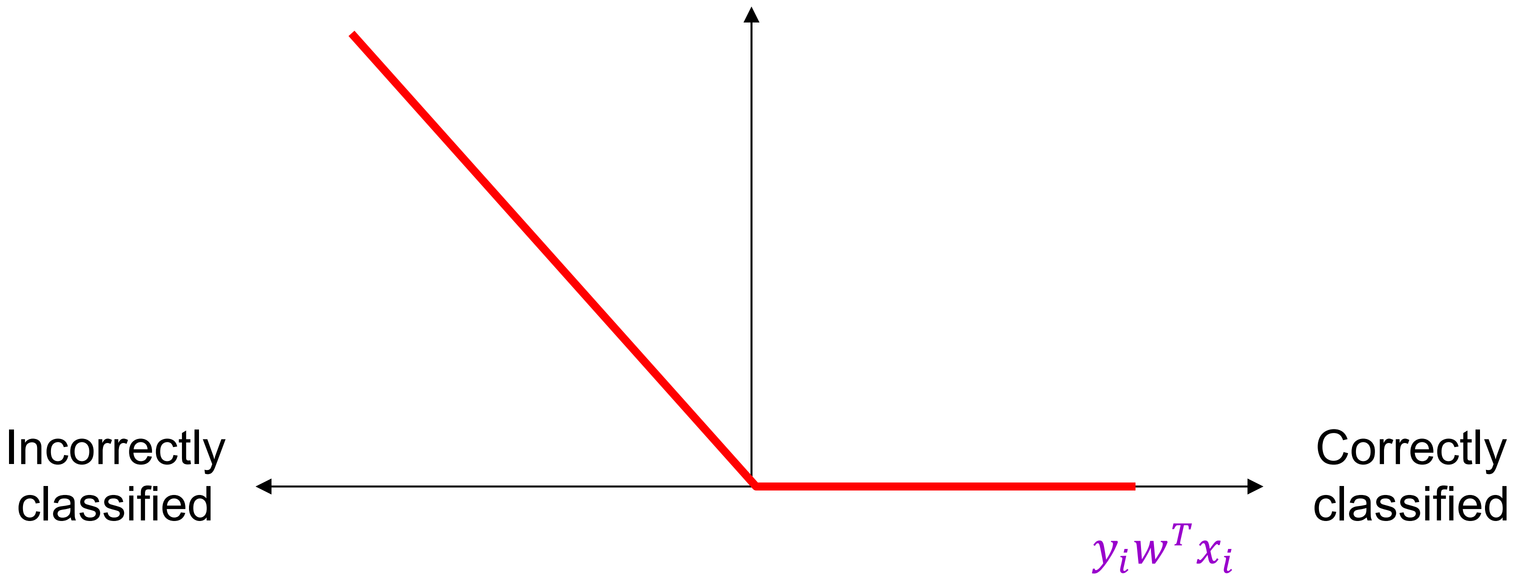
- Once again, there is no closed-form solution, so let's go straight to SGD

Deriving the perceptron update

- Let's differentiate the perceptron hinge loss:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

(Strictly speaking, this loss is not differentiable, so we need to find a *sub-gradient*)



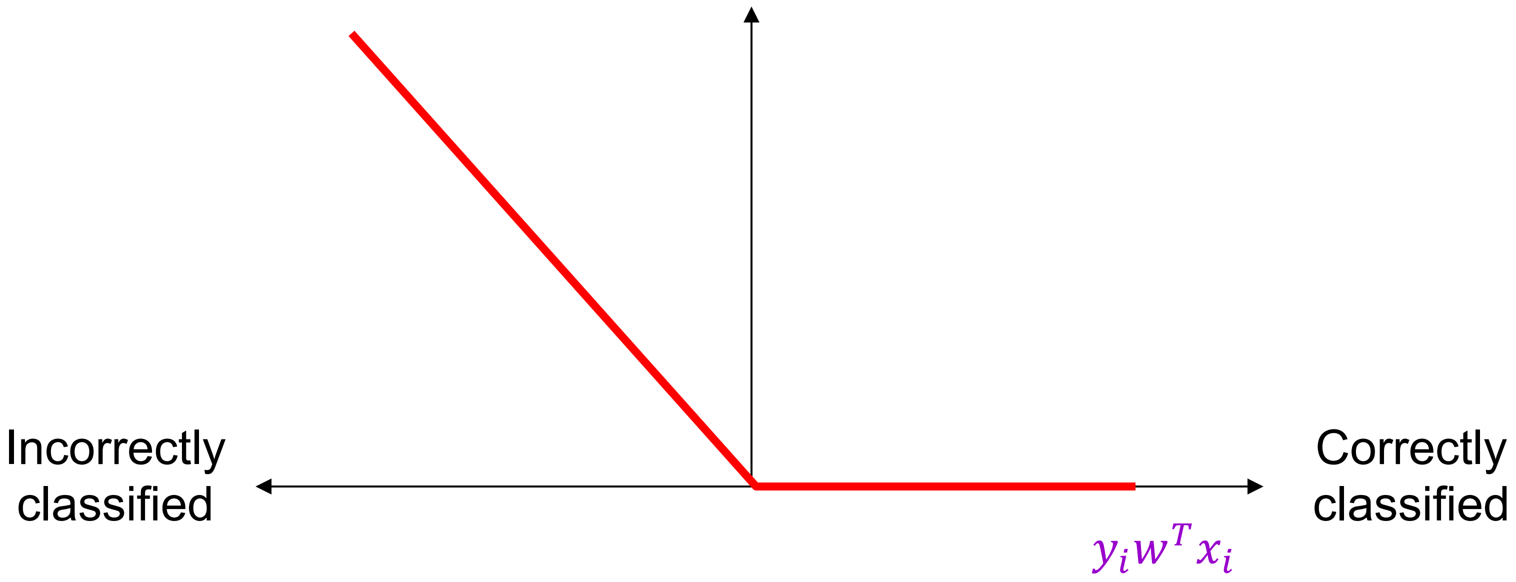
Deriving the perceptron update

- Let's differentiate the perceptron hinge loss:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

$$\nabla l(w, x_i, y_i) = -\mathbb{I}[y_i w^T x_i < 0] y_i x_i$$

$$\frac{d}{da} \max(0, a) =$$



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- We also used the chain rule: $\left[g_2\left(g_1(a)\right)\right]' = g_2'\left(g_1(a)\right) g_1'(a)$

Deriving the perceptron update

- Let's differentiate the perceptron hinge loss:

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$$\nabla l(w, x_i, y_i) = -\mathbb{I}[y_i w^T x_i < 0] y_i x_i$$

- Corresponding SGD update ($w \leftarrow w - \eta \nabla l(w, x_i, y_i)$):

$$w \leftarrow w + \eta\, \mathbb{I}[y_i w^T x_i < 0] y_i x_i$$

  - If x_i is correctly classified: do nothing
  - If x_i is incorrectly classified: $w \leftarrow w + \eta\, y_i x_i$

Understanding the perceptron update rule

- **Perceptron update rule:** If $y_i \neq \text{sgn}(w^T x_i)$ then update weights:

$$w \leftarrow w + \eta\, y_i x_i$$

- The raw response of the classifier changes to

$$w^T x_i + \eta\, y_i \|x_i\|^2$$

- How does the response change if $y_i = 1$?
  - The response $w^T x_i$ is initially *negative* and will be *increased*

- How does the response change if $y_i = -1$?
  - The response $w^T x_i$ is initially *positive* and will be *decreased*

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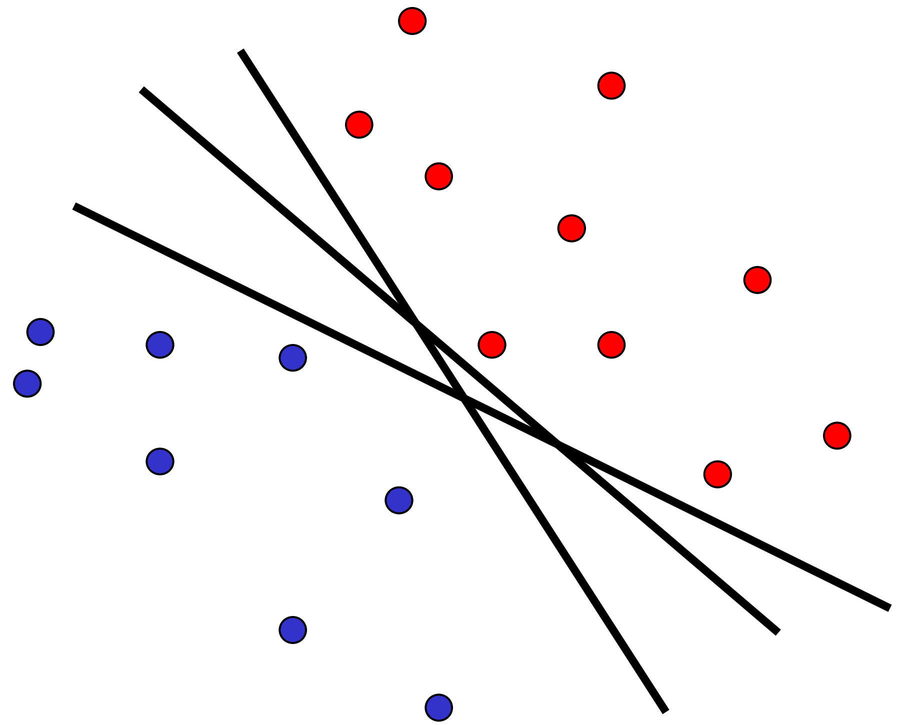
Support vector machines

- When the data is linearly separable, which of the many possible solutions should we prefer?

  - **Perceptron training algorithm:** no special criterion, solution depends on initialization

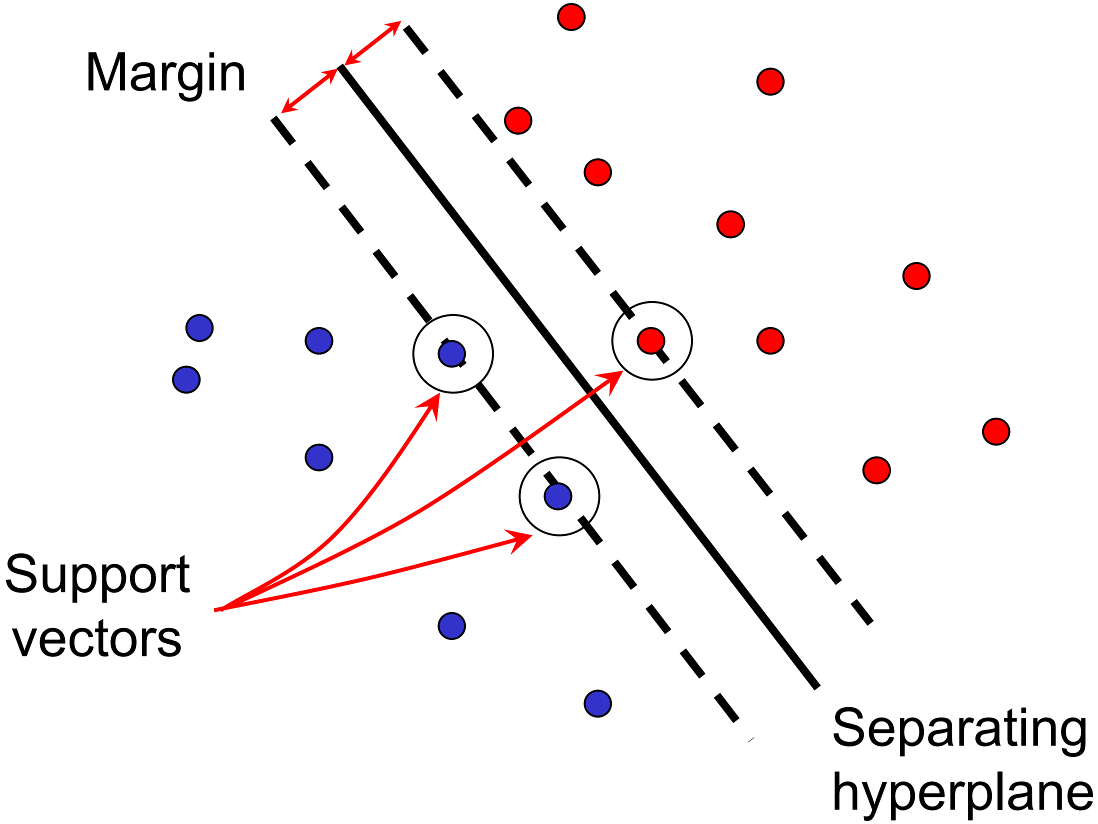


Support vector machines

- When the data is linearly separable, which of the many possible solutions should we prefer?

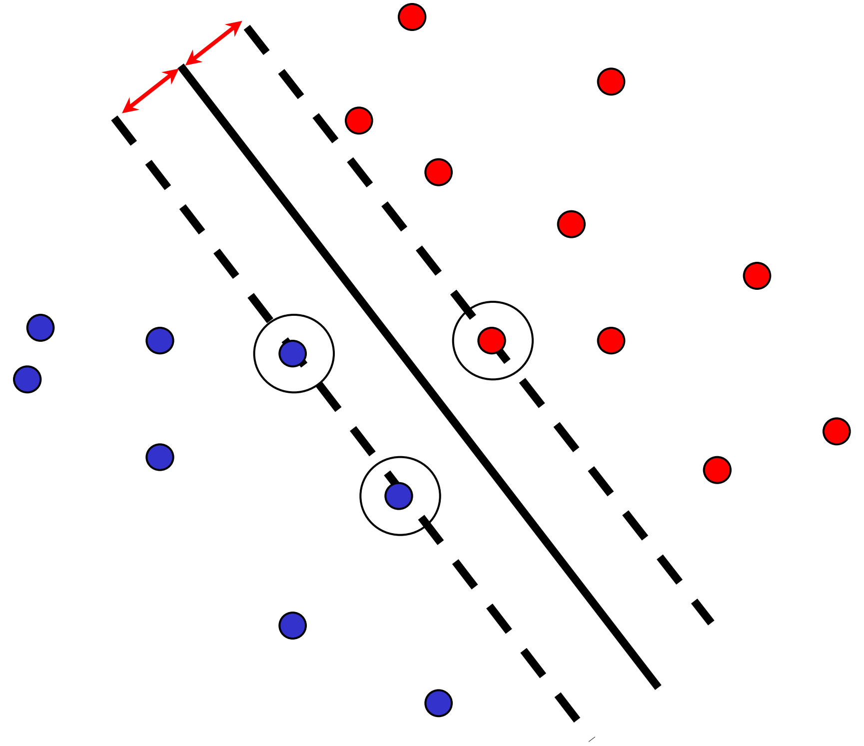
  - **Perceptron training algorithm:** no special criterion, solution depends on initialization

  - **SVM criterion:** maximize the *margin*, or distance between the hyperplane and the closest training example



Finding the maximum margin hyperplane

- We want to maximize the margin, or distance between the hyperplane $w^T x = 0$ and the closest training example x_0
- This distance is given by $\frac{|w^T x_0|}{\|w\|}$ (for derivation see, e.g., here)
- Assuming the data is linearly separable, we can fix the scale of w so that $y_i w^T x_i = 1$ for support vectors and $y_i w^T x_i \geq 1$ for all other points
- Then the margin is given by $\frac{1}{\|w\|}$



Finding the maximum margin hyperplane

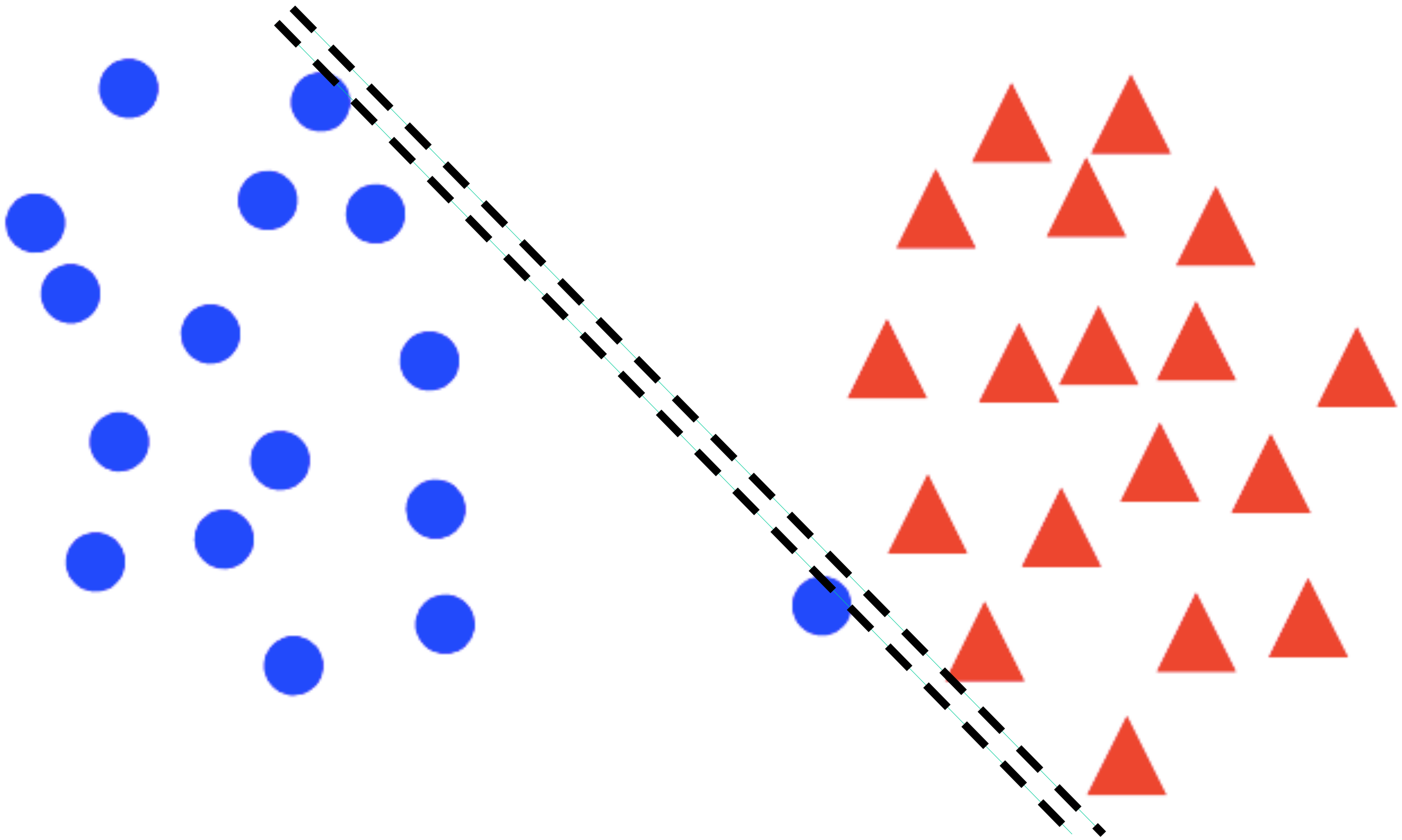
- We want to maximize margin $\frac{1}{\|w\|}$ while correctly classifying all training data: $y_i w^T x_i \geq 1$
- Equivalent problem:

$$\min_w \frac{1}{2}\|w\|^2 \quad \text{s.t.} \quad y_i w^T x_i \geq 1 \;\; \forall i$$

- This is a quadratic objective with linear constraints: convex optimization problem, global optimum can be found using well-studied methods

“Soft margin” formulation

- What about non-separable data?
- And even for separable data, we may prefer a larger margin with a few constraints violated



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"Soft margin" formulation

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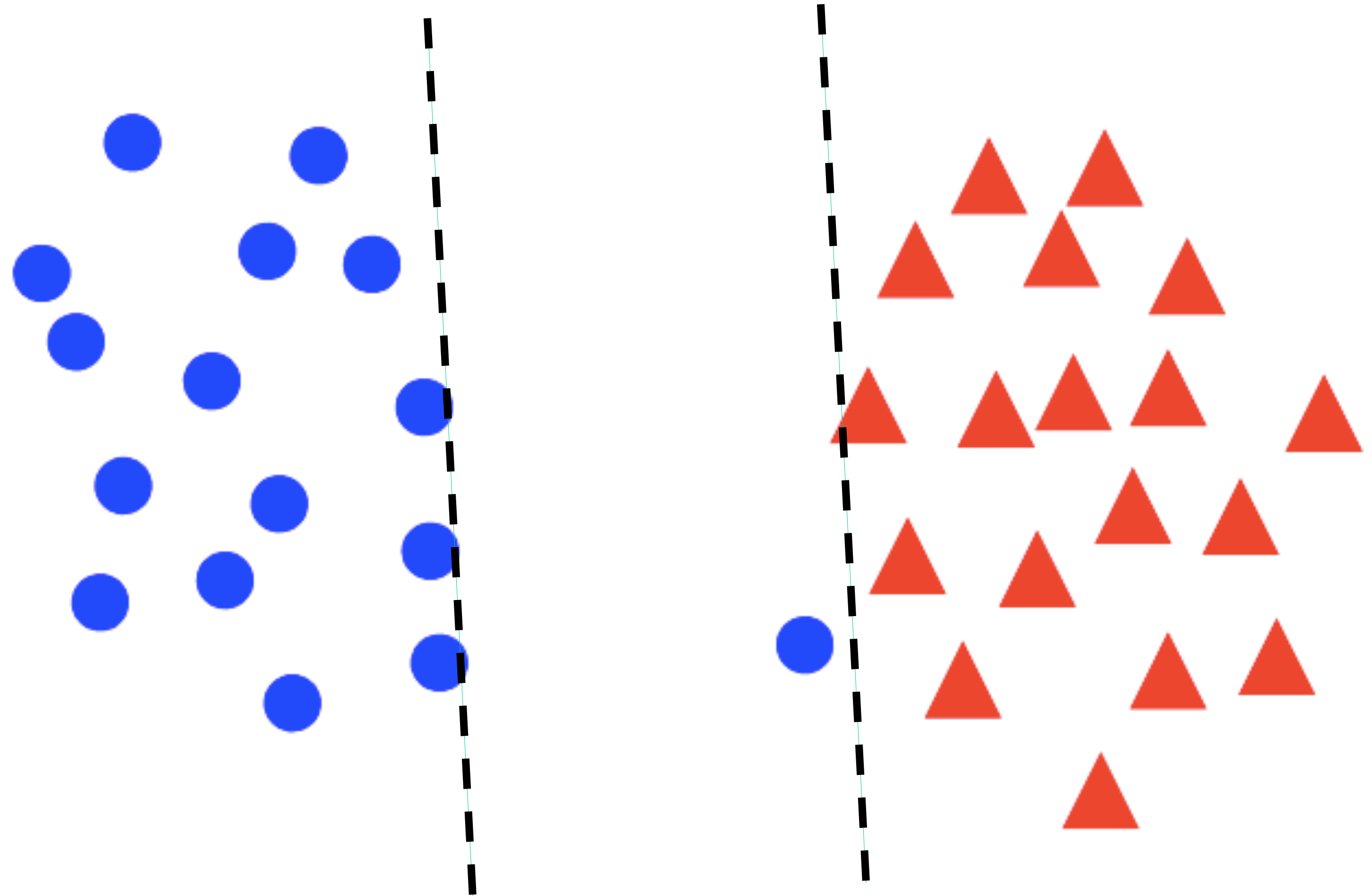

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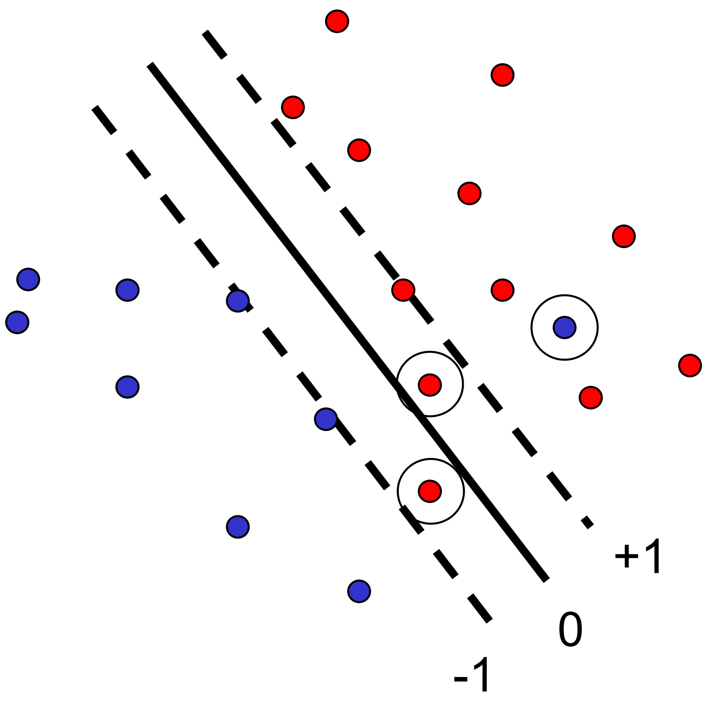
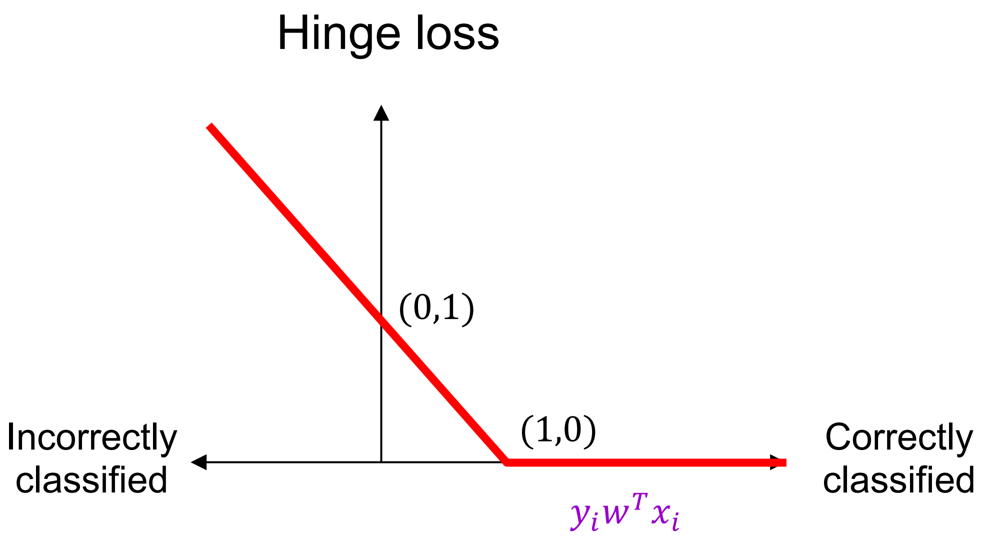
“Soft margin” formulation

- Penalize margin violations using SVM hinge loss:

$$\min_w \frac{\lambda}{2}\|w\|^2 \quad + \quad \sum_{i=1}^{n} \max[0, 1 - y_i w^T x_i]$$





"Soft margin" formulation

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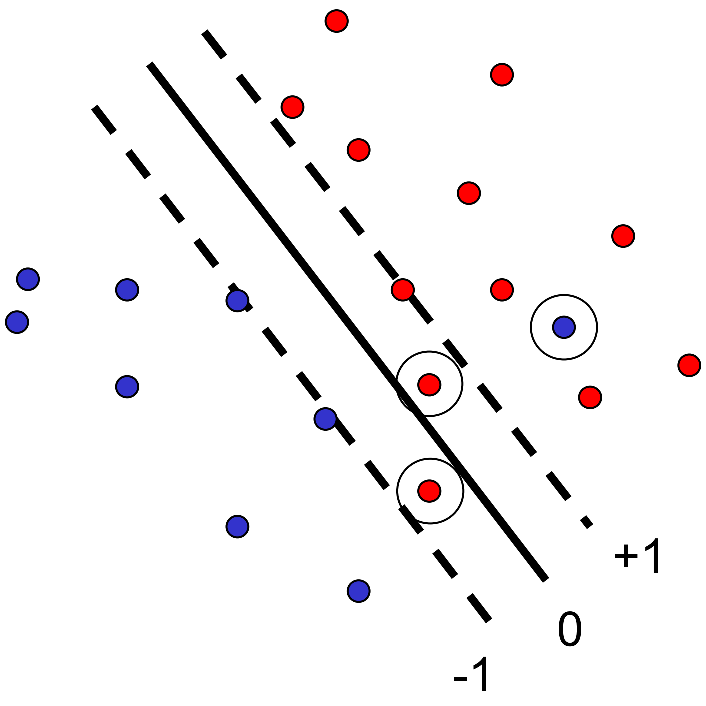

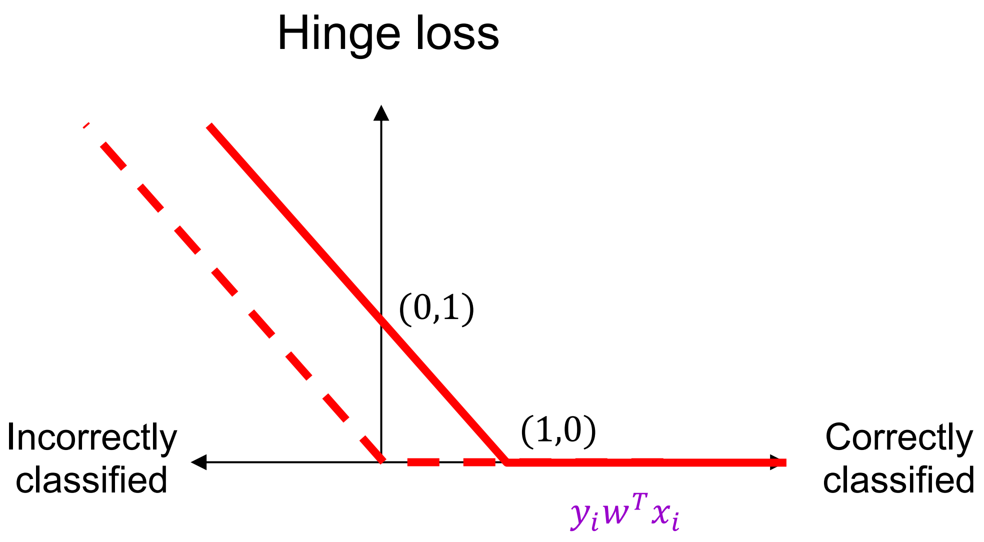

Recall hinge loss used by the perceptron update algorithm!

"Soft margin" formulation

- Penalize margin violations using SVM hinge loss:

$$\underbrace{\min_w \frac{\lambda}{2}\|w\|^2}_{\text{Maximize margin – a.k.a. } \textit{regularization}} \quad + \quad \underbrace{\sum_{i=1}^{n} \max[0, 1 - y_i w^T x_i]}_{\text{Minimize misclassification loss}}$$

SGD update for SVM

$$l(w, x_i, y_i) = \frac{\lambda}{2n}\|w\|^2 + \max[0, 1 - y_i w^T x_i]$$

$$\nabla l(w, x_i, y_i) = \frac{\lambda}{n} w - \mathbb{I}[y_i w^T x_i < 1] y_i x_i$$

Recall: $\frac{d}{da}\max(0, a) = \mathbb{I}[a > 0]$

SGD update for SVM

$$l(w, x_i, y_i) = \frac{\lambda}{2n}\|w\|^2 + \max[0, 1 - y_i w^T x_i]$$

$$\nabla l(w, x_i, y_i) = \frac{\lambda}{n} w - \mathbb{I}[y_i w^T x_i < 1] y_i x_i$$

- SGD update:
  - If $y_i w^T x_i \geq 1$: $w \leftarrow w - \eta \frac{\lambda}{n} w$
  - If $y_i w^T x_i < 1$: $w \leftarrow w + \eta \left(y_i x_i - \frac{\lambda}{n} w \right)$

S. Shalev-Schwartz et al., Pegasos: Primal Estimated sub-GrAdient SOlver for SVM, *Mathematical Programming*, 2011

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- General recipe: data loss, regularization

General recipe

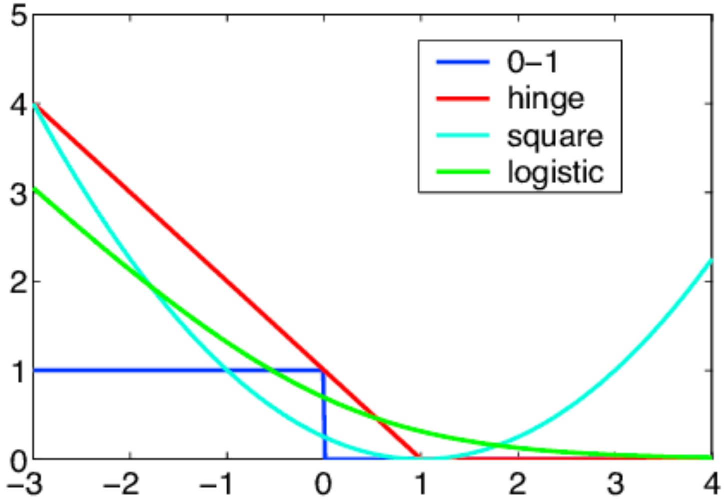
- Find parameters w that minimize the sum of a *regularization loss* and a *data loss*:

$$\hat{L}(w) = \lambda R(w) + \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i)$$

empirical loss — regularization — data loss

L2 regularization:

$$R(w) = \frac{1}{2}\|w\|_2^2$$



Closer look at L2 regularization

- Regularized objective: $\hat{L}(w) = \frac{\lambda}{2}\|w\|_2^2 + \sum_{i=1}^{n} l(w, x_i, y_i)$
- Gradient of objective:

$$\nabla\hat{L}(w) = \lambda w + \sum_{i=1}^{n} \nabla l(w, x_i, y_i)$$

- SGD update:

$$w \leftarrow w - \eta\left(\frac{\lambda}{n} w + \nabla l(w, x_i, y_i)\right)$$

$$w \leftarrow \left(1 - \frac{\eta\lambda}{n}\right) w - \eta\nabla l(w, x_i, y_i)$$

- Interpretation: weight decay

General recipe

- Find parameters w that minimize the sum of a *regularization loss* and a *data loss*:

$$\hat{L}(w) = \lambda R(w) + \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i)$$

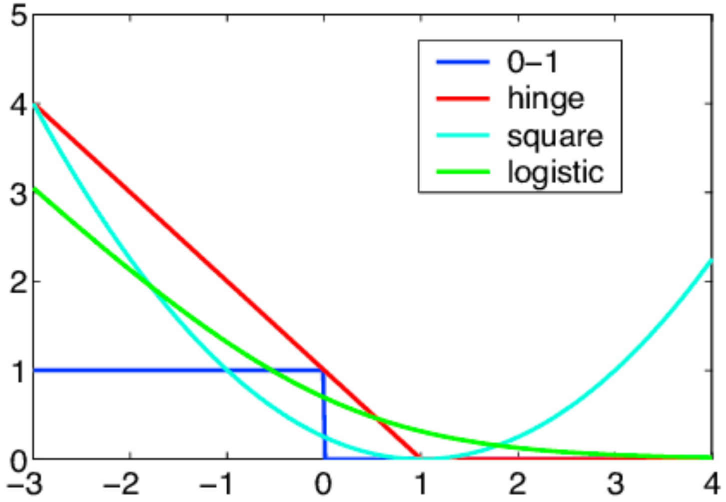
empirical loss — regularization — data loss

L2 regularization:

$$R(w) = \frac{1}{2}\|w\|_2^2$$

L1 regularization:

$$R(w) = \|w\|_1$$



Closer look at L1 regularization

- Regularized objective:

$$\hat{L}(w) = \lambda \|w\|_1 + \sum_{i=1}^{n} l(w, x_i, y_i)$$

$$= \lambda \sum_{d} \left| w^{(d)} \right| + \sum_{i=1}^{n} l(w, x_i, y_i)$$

- Gradient: $\nabla \hat{L}(w) = \lambda \operatorname{sgn}(w) + \sum_{i=1}^{n} \nabla l(w, x_i, y_i)$

  (here sgn is an elementwise function)

- SGD update:

$$w \leftarrow w - \frac{\eta \lambda}{n} \operatorname{sgn}(w) - \eta \nabla l(w, x_i, y_i)$$

- Interpretation: encouraging sparsity

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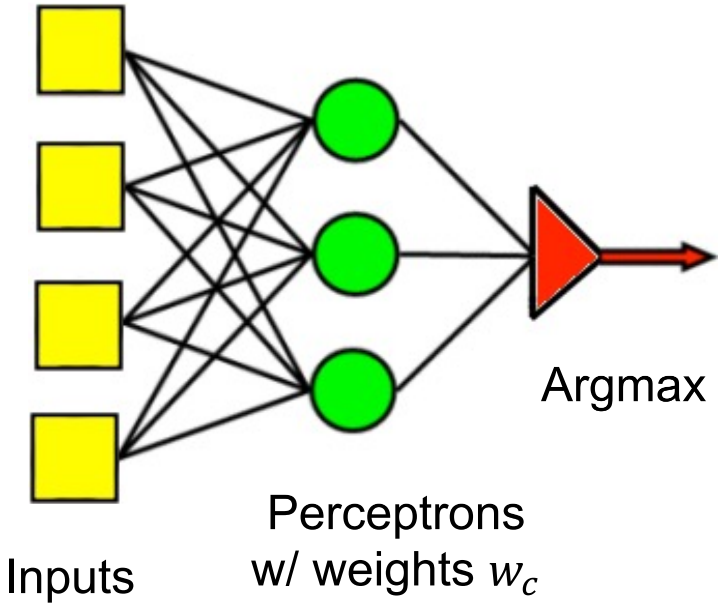
One-vs-all classification

- Let $y \in \{1, \dots, C\}$
- Learn C scoring functions $f_1, f_2, \dots, f_C$
- Classify x to class $\hat{y} = \mathrm{argmax}_c\ f_c(x)$
- Let's start with multi-class perceptrons:

$$f_c(x) = w_c^T x$$



Multi-class perceptrons

- Multi-class perceptrons: $f_c(x) = w_c^T x$
- Let W be the matrix with rows w_c
- What loss should we use for multi-class classification?

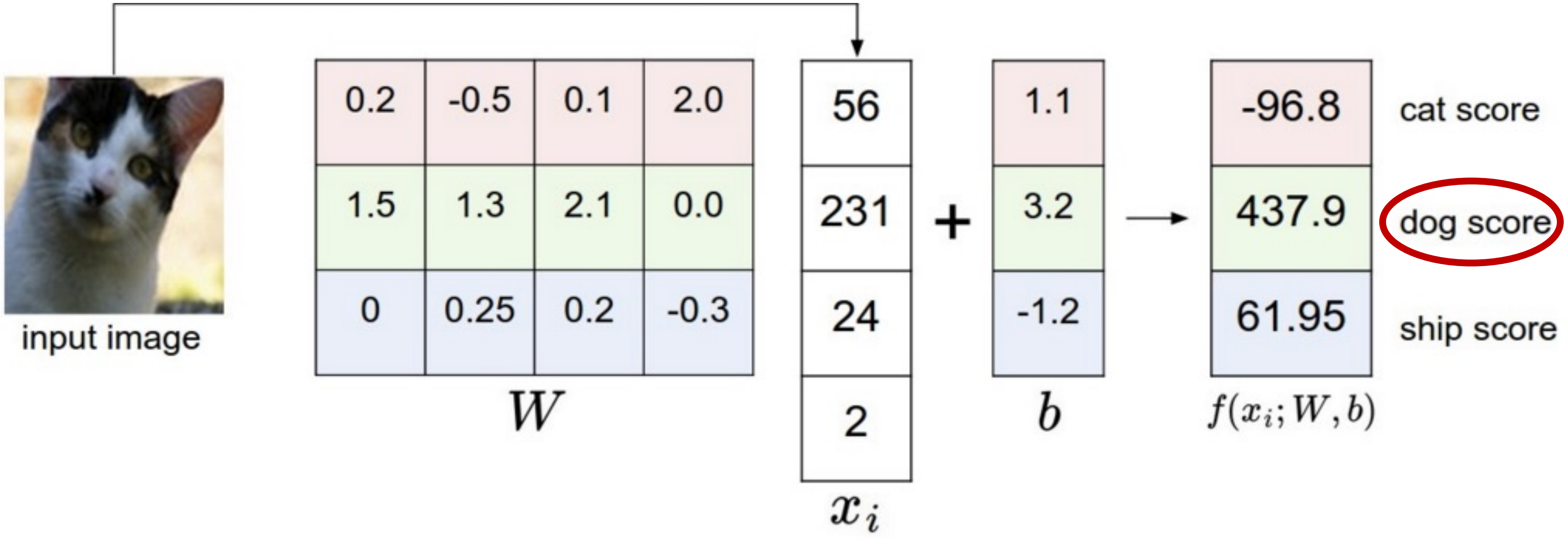


Figure source: [Stanford 231n]()

Multi-class perceptrons

- Multi-class perceptrons: $f_c(x) = w_c^T x$
- Let W be the matrix with rows w_c
- What loss should we use for multi-class classification?
- For (x_i, y_i), let the loss be the *sum of hinge losses* associated with predictions for all *incorrect* classes:

$$l(W, x_i, y_i) = \sum_{c \neq y_i} \max[0, w_c^T x_i - w_{y_i}^T x_i]$$

Score for correct class (y_i)
has to be greater than the
score for the incorrect class (c)

Multi-class perceptrons

$$l(W, x_i, y_i) = \sum_{c \neq y_i} \max[0, w_c^T x_i - w_{y_i}^T x_i]$$

- Gradient w.r.t. w_{y_i}:

$$-\sum_{c \neq y_i} \mathbb{I}\,[w_c^T x_i > w_{y_i}^T x_i] x_i$$

Recall: $\frac{d}{da} \max(0, a) = \mathbb{I}[a > 0]$

Multi-class perceptrons

$$l(W, x_i, y_i) = \sum_{c \neq y_i} \max[0, w_c^T x_i - w_{y_i}^T x_i]$$

- Gradient w.r.t. w_{y_i}:

$$-\sum_{c \neq y_i} \mathbb{I}\,[w_c^T x_i > w_{y_i}^T x_i] x_i$$

- Gradient w.r.t. w_c, $c \neq y_i$:

$$\mathbb{I}[w_c^T x_i > w_{y_i}^T x_i] x_i$$

- Update rule: for each c s.t. $w_c^T x_i > w_{y_i}^T x_i$:

$$w_{y_i} \leftarrow w_{y_i} + \eta x_i$$
$$w_c \leftarrow w_c - \eta x_i$$

Multi-class perceptrons

- Update rule: for each c s.t. $w_c^T x_i > w_{y_i}^T x_i$:

$$w_{y_i} \leftarrow w_{y_i} + \eta x_i$$
$$w_c \leftarrow w_c - \eta x_i$$

- Is this equivalent to training C independent one-vs-all classifiers?

input image

	Independent	Multi-class
Cat score: 65.1	Do nothing	Increase
Dog score: 101.4	Decrease	Decrease
Ship score: 24.9	Decrease	Do nothing

Multi-class SVM

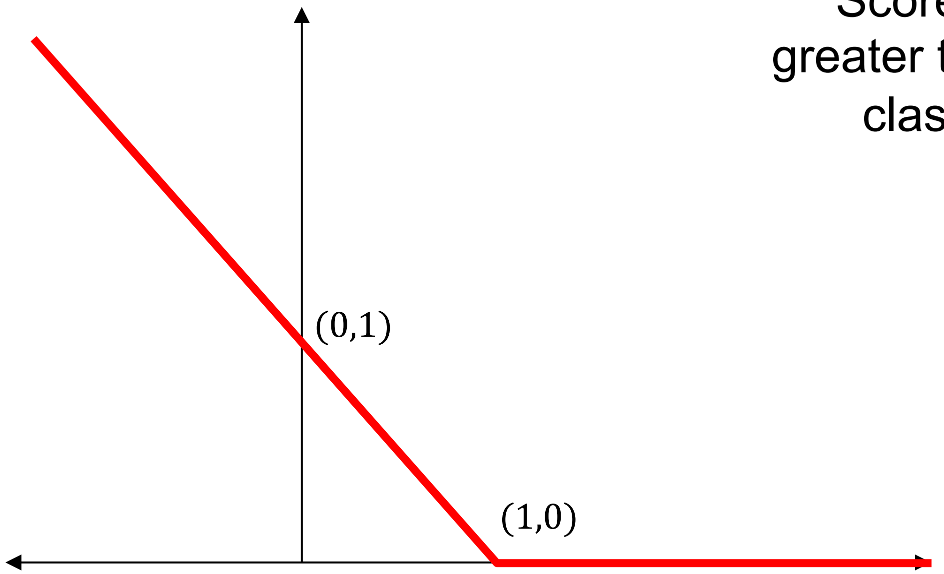
- Recall single-class SVM loss:

$$l(w, x_i, y_i) = \frac{\lambda}{2n}\|w\|^2 + \max[0, 1 - y_i w^T x_i]$$

- Generalization to multi-class:

$$l(W, x_i, y_i) = \frac{\lambda}{2n}\|W\|^2 + \sum_{c \neq y_i} \max[0, 1 - w_{y_i}^T x_i + w_c^T x_i]$$

Score for correct class has to be greater than the score for the incorrect class *by at least a margin of* 1



Score for correct class – score for incorrect class

Source: [Stanford 231n]

Multi-class SVM

$$l(W, x_i, y_i) = \frac{\lambda}{2n}\|W\|^2 + \sum_{c \neq y_i} \max[0, 1 - w_{y_i}^T x_i + w_c^T x_i]$$

- Gradient w.r.t. w_{y_i}:

$$\frac{\lambda}{n} w_{y_i} - \sum_{c \neq y_i} \mathbb{I}[w_{y_i}^T x_i - w_c^T x_i < 1] x_i$$

- Gradient w.r.t. w_c, $c \neq y_i$:

$$\frac{\lambda}{n} w_c + \mathbb{I}[w_{y_i}^T x_i - w_c^T x_i < 1] x_i$$

- Update rule (almost* equivalent to above):
  - For each $c \neq y_i$ s.t. $w_{y_i}^T x_i - w_c^T x_i < 1$: $w_{y_i} \leftarrow w_{y_i} + \eta x_i, \;\; w_c \leftarrow w_c - \eta x_i$
  - For $c = 1, \ldots, C$: $w_c \leftarrow \left(1 - \eta \frac{\lambda}{n}\right) w_c$

Softmax

- We want to squash the vector of responses $(f_1, \ldots, f_c)$ into a vector of "probabilities":

$$\text{softmax}(f_1, \ldots, f_c) = \left(\frac{\exp(f_1)}{\sum_j \exp(f_j)}, \ldots, \frac{\exp(f_c)}{\sum_j \exp(f_j)} \right)$$

- The entries are between 0 and 1 and sum to 1
- If one of the inputs is much larger than the others, then the corresponding softmax value will be close to 1 and others will be close to 0

Softmax and sigmoid

- For two classes:

$$\text{softmax}(f, -f) = \left(\frac{\exp(f)}{\exp(f) + \exp(-f)}, \frac{\exp(-f)}{\exp(f) + \exp(-f)}\right)$$
$$= \left(\frac{1}{1+\exp(-2f)}, \frac{1}{\exp(2f)+1}\right)$$
$$= (\sigma(2f), \sigma(-2f))$$

- Thus, softmax is the generalization of sigmoid for more than two classes

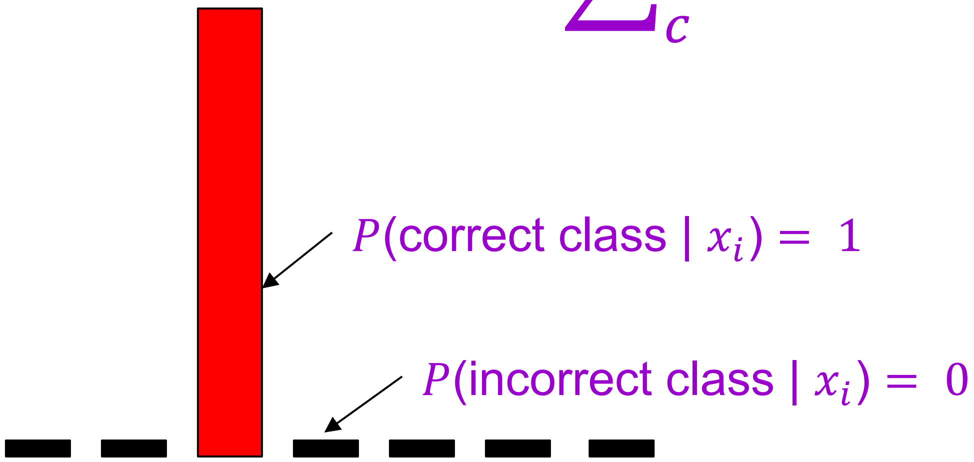
Cross-entropy loss

- It is natural to use negative log likelihood loss with softmax:

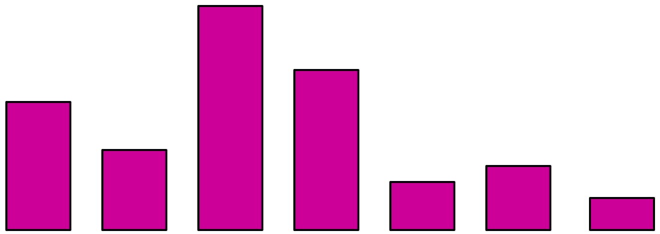
$$l(W, x_i, y_i) = -\log P_W(y_i|x_i) = -\log\left(\frac{\exp(w_{y_i}^T x_i)}{\sum_j \exp(w_j^T x_i)}\right)$$

- This is also the *cross-entropy* between the “empirical” distribution $\hat{P}(c|x_i) = \mathbb{I}[c = y_i]$ and “estimated” distribution $P_W(c|x_i)$:

$$-\sum_c \hat{P}(c|x_i) \log P_W(c|x_i)$$

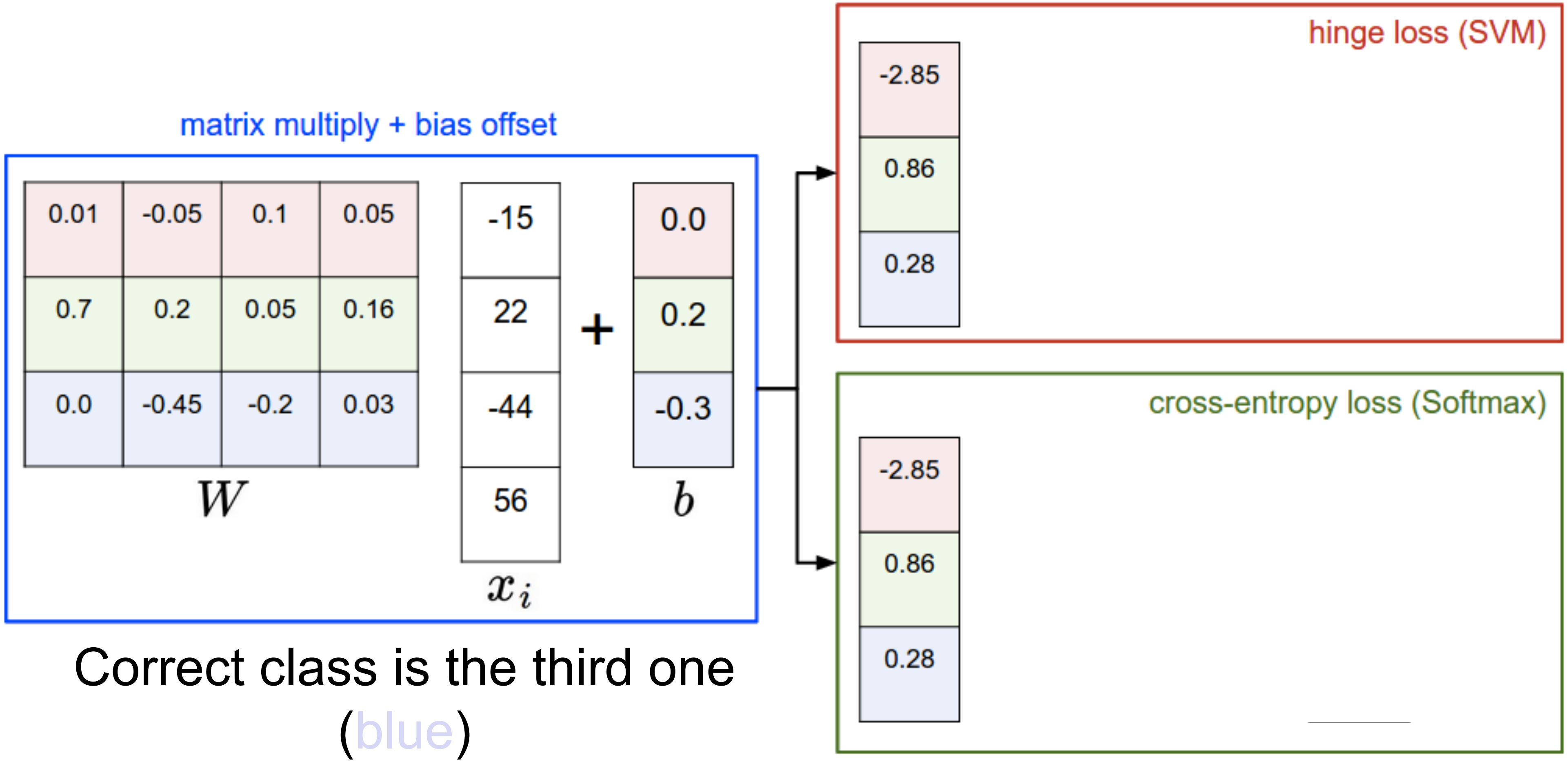


Empirical distribution $\hat{P}(c|x_i)$



Estimated distribution $P_W(c|x_i)$

SVM loss vs. cross-entropy loss



Correct class is the third one (blue)

Source: [Stanford 231n]

SGD with cross-entropy loss

$$l(W, x_i, y_i) = -\log P_W(y_i|x_i) = -\log\left(\frac{\exp(w_{y_i}^T x_i)}{\sum_j \exp(w_j^T x_i)}\right)$$

$$= -w_{y_i}^T x_i + \log\left(\sum_j \exp(w_j^T x_i)\right)$$

- Gradient w.r.t. w_{y_i}:

$$-x_i + \frac{\exp(w_{y_i}^T x_i) x_i}{\sum_j \exp(w_j^T x_i)} = (P_W(y_i|x_i) - 1) x_i$$

- Gradient w.r.t. w_c, $c \neq y_i$:

$$\frac{\exp(w_c^T x_i) x_i}{\sum_j \exp(w_j^T x_i)} = P_W(c|x_i) x_i$$

SGD with cross-entropy loss

- Gradient w.r.t. w_{y_i}: $(P_W(y_i|x_i) - 1)x_i$
- Gradient w.r.t. w_c, $c \neq y_i$: $P_W(c|x_i)x_i$
- Update rule:
  - For y_i:
    $$w_{y_i} \leftarrow w_{y_i} + \eta\big(1 - P_W(y_i|x_i)\big)x_i$$
  - For $c \neq y_i$:
    $$w_c \leftarrow w_c - \eta P_W(c|x_i)x_i$$

Softmax trick: Avoiding overflow

- Exponentiated values $\exp(f_c)$ can become very large and cause overflow
- Note that adding the same constant to all softmax inputs (*logits*) does not change the output of the softmax:

$$\frac{\exp(f_c)}{\sum_j \exp(f_j)} = \frac{K \exp(f_c)}{\sum_j K \exp(f_j)} = \frac{\exp(f_c + \log K)}{\sum_j \exp(f_j + \log K)}$$

- Then we can let $\log K = -\max_j f_j$ (i.e., make largest input to softmax be 0)

Softmax trick: Temperature scaling

- Suppose we divide every input to the softmax by the same constant T:

$$\text{softmax}(f_1, \dots, f_c; T) = \left(\frac{\exp(f_1/T)}{\sum_j \exp(f_j/T)}, \dots, \frac{\exp(f_c/T)}{\sum_j \exp(f_j/T)} \right)$$

- What does this accomplish?
  - Prior to normalization, each entry $\exp(f_1)$ is raised to the power $1/T$
  - If T is close to 0, the largest entry will dominate and output distribution will tend to *one-hot*
  - If T is high, output distribution will tend to uniform

Softmax trick: Temperature scaling

Low temperature: More concentrated distribution

Higher temperature: More uniform distribution

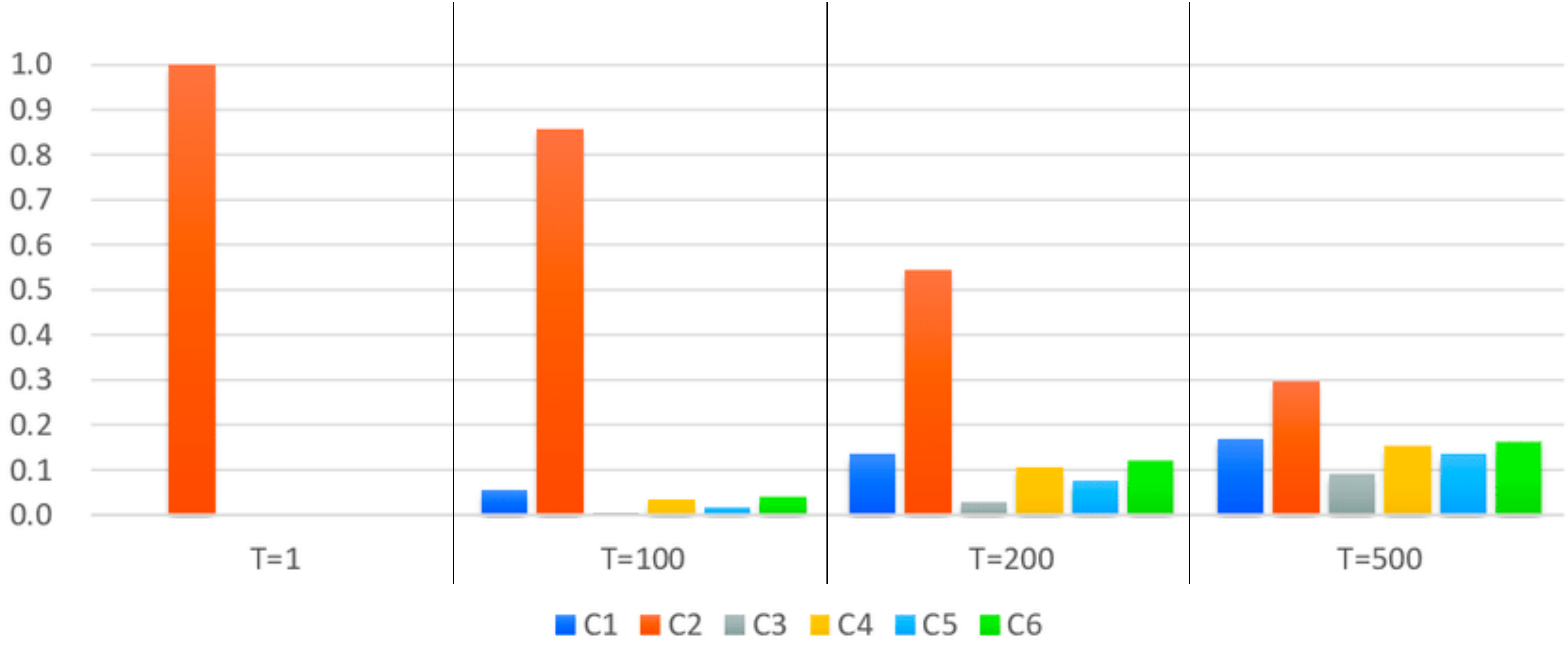


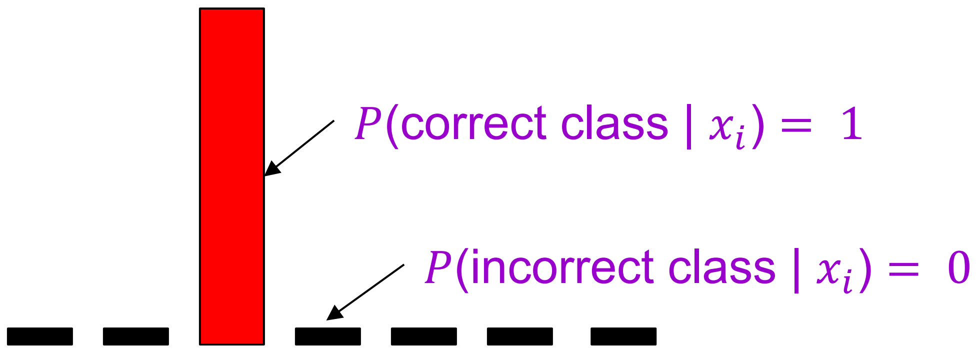
Figure source

Softmax trick: Label smoothing

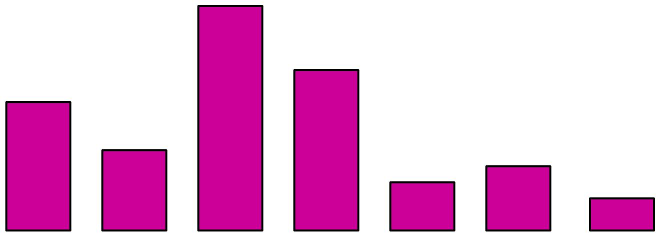
- Recall: cross-entropy loss measures the difference between the "observed" label distribution $\hat{P}(c|x_i)$ and "estimated" distribution $P_W(c|x_i)$:

$$-\sum_c \hat{P}(c|x_i) \log P_W(c|x_i)$$

"Hard" prediction targets



Empirical distribution $\hat{P}(c|x_i)$



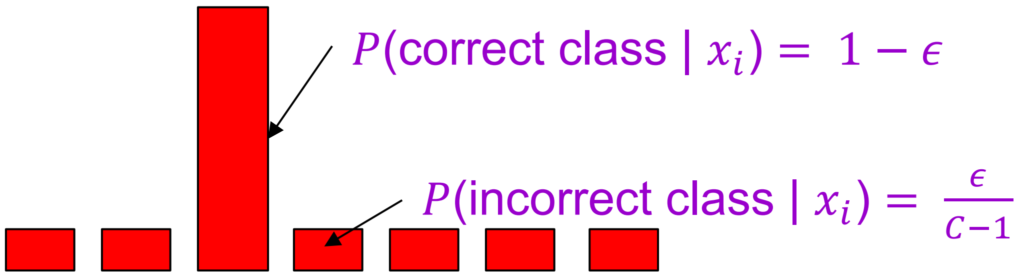
Estimated distribution $P_W(c|x_i)$

Softmax trick: Label smoothing

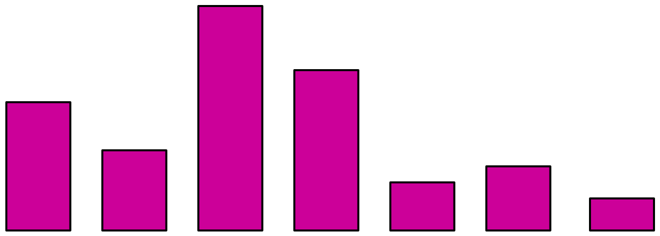
- Recall: cross-entropy loss measures the difference between the "observed" label distribution $\hat{P}(c|x_i)$ and "estimated" distribution $P_W(c|x_i)$:

$$-\sum_c \hat{P}(c|x_i) \log P_W(c|x_i)$$

"Soft" prediction targets



Empirical distribution $\hat{P}(c|x_i)$



Estimated distribution $P_W(c|x_i)$

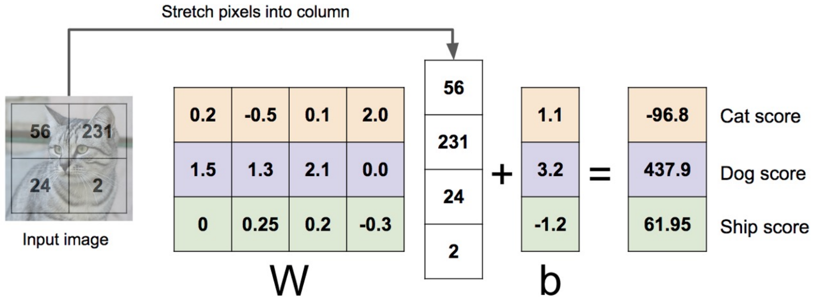
Softmax trick: Label smoothing

- When using softmax loss, replace hard 1 and 0 prediction targets with "soft" targets of $1 - \epsilon$ and $\frac{\epsilon}{C-1}$
- Why is this a good idea?
  - A form of regularization to avoid overly confident predictions, account for label noise

Recap: Three ways to think about linear classifiers

Algebraic Viewpoint

$$f_W(x) = Wx$$

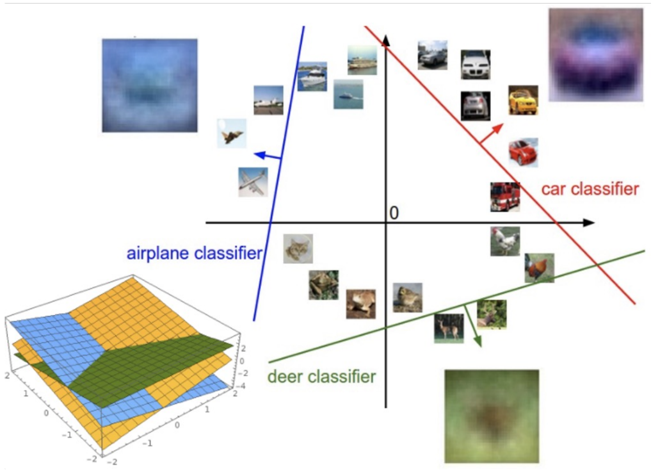


Visual Viewpoint

One template
per class

Geometric Viewpoint

Hyperplanes
cutting up space



Source: [J. Johnson]