COMP90051

Workshop Week 07

About the Workshops

- 7 sessions in total
  - Tue 12:00-13:00 AH211
  - Tue 12:00-13:00 AH108 *
  - Tue 13:00-14:00 AH210
  - Tue 16:15-17:15 AH109
  - Tue 17:15-18:15 AH236 *
  - Tue 18:15-19:15 AH236 *
  - Fri 14:15-15:15 AH211

About the Workshops

- Homepage
  - https://trevorcohn.github.io/comp90051-2017/workshops

- Solutions will be released on next Friday (a week later).

Syllabus

1	Introduction; Probability theory	Probabilistic models; Parameter fitting	
2	Linear regression; Intro to regularization	Logistic regression; Basis expansion	
3	Optimization; Regularization	Perceptron	
4	Backpropagation	CNNs; Auto-encoders	
5	Hard-margin SVMs	Soft-margin SVMs	←
6	Kernel methods	Ensemble Learning	←
7	Clustering	EM algorithm	
8	Dimensionality reduction; Principal component analysis	Multidimensional scaling; Spectral clustering	
9	Bayesian fundamentals	Bayesian inference with conjugate priors	
10	PGMs, fundamentals	Conditional independence	
11	PGMs, inference	Belief propagation	
12	Statistical inference; Apps	Subject review	

Outline

- Review the lecture, background knowledge, etc.
  - Bagging
    - OOB score
  - SVM
    - Hard-margin & Soft-margin
    - Comparison with logistic regression, perceptron
  - Kernel method
- Run ipython notebooks

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Bagging (bootstrap aggregating)

- A model averaging approach

- Given a standard training set
- Bootstrap the standard training set
  - To generate m new training sets
  - Bootstrap = sample uniformly and with replacement
- Train m base models on the above m training sets
- Aggregate the m base models to make predictions
  - By voting (classification) or averaging (regression)

Sample without replacement

Iteration	Choose from	Generate	Sample
1	[1 2 3 4 5 6 7 8 9]	[4]	[4]
2	[1 2 3 5 6 7 8 9]	[1]	[4,1]
3	[2 3 5 6 7 8 9]	[3]	[4,1,3]
4	[2 5 6 7 8 9]	[2]	[4,1,3,2]

Sample with replacement

Iteration	Choose from	Generate	Sample
1	[1 2 3 4 5 6 7 8 9]	[4]	[4]
2	[1 2 3 4 5 6 7 8 9]	[1]	[4,1]
3	[1 2 3 4 5 6 7 8 9]	[4]	[4,1,4]
4	[1 2 3 4 5 6 7 8 9]	[1]	[4,1,4,1]

Original dataset: $\{(\boldsymbol{x}_i, y_i)\}, i = 1,2, \ldots, 9$

Model	Training set
m1	[6 3 6 2 7 4 8 3 4]
m2	[4 7 1 5 4 5 1 1 4]
m3	[7 2 8 4 4 3 7 1 1]
m4	[8 2 9 3 9 3 2 5 9]

- To make a prediction for x

$$\hat{y} = \frac{1}{4}\{m1.predict(x) + m2.predict(x) + m3.predict(x) + m4.predict(x)\}$$

OOB: out-of-bag

Model	Training set	OOB
m1	[6 3 6 2 7 4 8 3 4]	[1 5 9]
m2	[4 7 1 5 4 5 1 1 4]	[2 3 6 8 9]
m3	[7 2 8 4 4 3 7 1 1]	[5 6 9]
m4	[8 2 9 3 9 3 2 5 9]	[1 4 6 7]

- To make a prediction for x

$$\hat{y} = \frac{1}{4}\{m1.predict(x) + m2.predict(x) + m3.predict(x) + m4.predict(x)\}$$

$\tilde{y}_i$: aggregation of models haven't seen $\boldsymbol{x}_i$

Model	Training set	OOB
m1	[6 3 6 2 7 4 8 3 4]	[1 5 9]
m2	[4 7 1 5 4 5 1 1 4]	[2 3 6 8 9]
m3	[7 2 8 4 4 3 7 1 1]	[5 6 9]
m4	[8 2 9 3 9 3 2 5 9]	[1 4 6 7]

$$\tilde{y}_1 = \frac{1}{2}\{m1.predict(\boldsymbol{x}_1) + m4.predict(\boldsymbol{x}_1)\}$$

$$\tilde{y}_2 = m2.predict(\boldsymbol{x}_2) \qquad \tilde{y}_3 = m2.predict(\boldsymbol{x}_3)$$

$$\tilde{y}_4 = m4.predict(\boldsymbol{x}_4) \qquad \tilde{y}_5 = m3.predict(\boldsymbol{x}_5)$$

$$\tilde{y}_6 = \frac{1}{3}\{m2.predict(\boldsymbol{x}_6) + m3.predict(\boldsymbol{x}_6) + m4.predict(\boldsymbol{x}_6)\}$$

$$\tilde{y}_7 = m4.predict(\boldsymbol{x}_7) \qquad \tilde{y}_8 = m2.predict(\boldsymbol{x}_8)$$

$$\tilde{y}_9 = \frac{1}{3}\{m1.predict(\boldsymbol{x}_9) + m2.predict(\boldsymbol{x}_9) + m3.predict(\boldsymbol{x}_9)\}$$

OOB score (regression)

- OOB mean squared error

$$MSE_{OOB} = \frac{1}{|D_{train}|} \sum_{(x_i, y_i) \in D_{train}} (y_i - \tilde{y}_i)^2$$

- Mean squared error on a validation set

$$MSE_{val} = \frac{1}{|D_{val}|} \sum_{(x_i, y_i) \in D_{val}} (y_i - \hat{y}_i)^2$$

- OOB score is an alternative to the score on validation set

Bagging

- Can be used with any type of method
- Usually applied to decision tree method

- In sklearn:

```
>>> from sklearn.ensemble import BaggingClassifier
>>> from sklearn.neighbors import KNeighborsClassifier
>>> bagging = BaggingClassifier(KNeighborsClassifier(),
...                             max_samples=0.5, max_features=0.5)
```

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SVM

- Hard-margin

$$\min_{\boldsymbol{w},b} \frac{1}{2}||w||^2$$

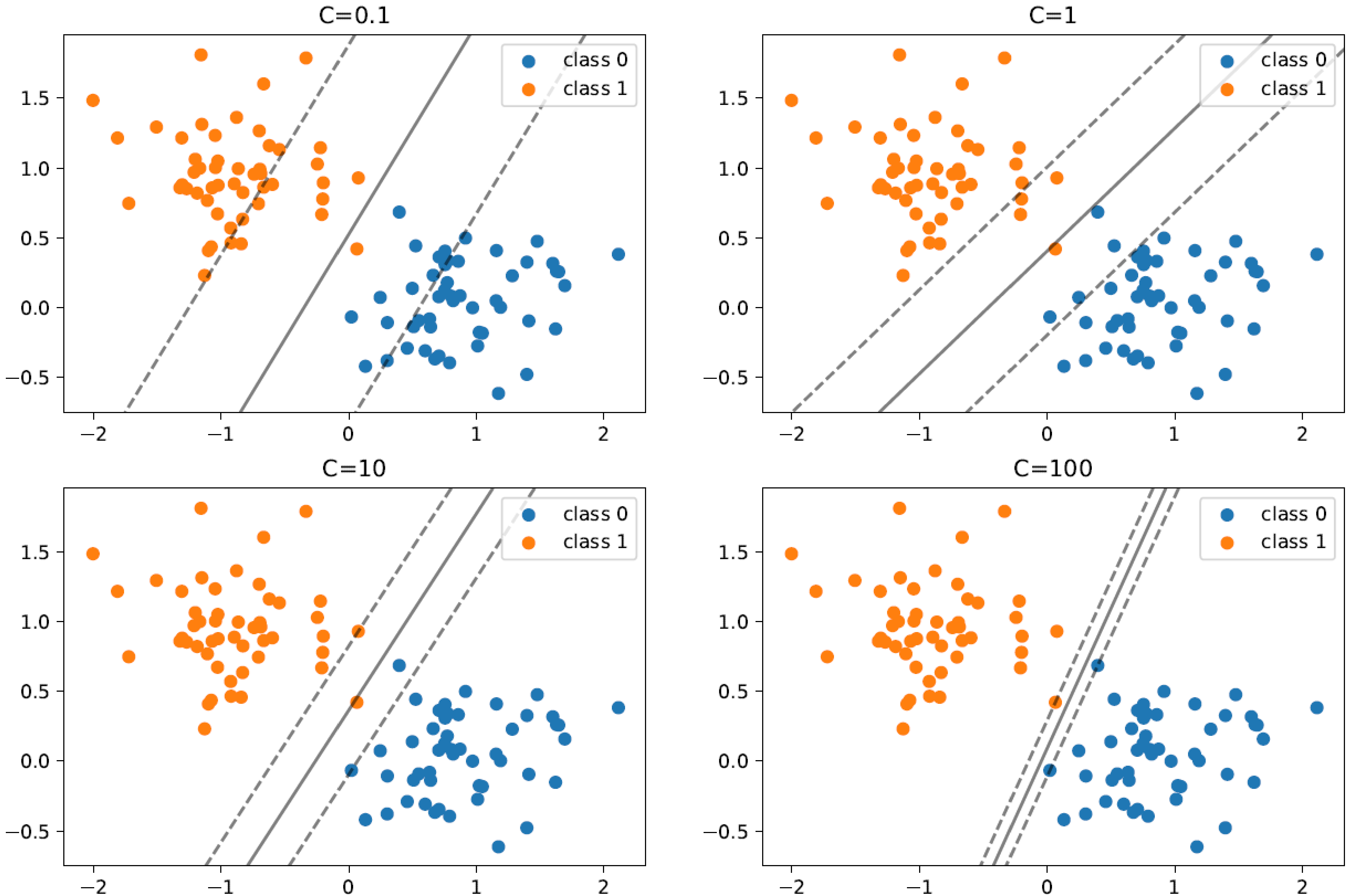
$$s.t. \quad y_i(\boldsymbol{w}^T\boldsymbol{x}_i + b) \geq 1$$

- Soft-margin

$$\min_{\boldsymbol{w},b} \frac{1}{2}||w||^2 + C\sum_{i=0}^{n} \max\left(0, 1 - y_i(\boldsymbol{w}^T\boldsymbol{x}_i + b)\right)$$

- Hard-margin $\Leftrightarrow C \to +\infty$

SVM - different C values



SVM and Perceptron

$$s_i = \boldsymbol{w}^T \boldsymbol{x}_i + b$$

- Hinge loss

$$L(\boldsymbol{x}_i, y_i) = \max(0, 1 - y_i s_i)$$

- Perceptron loss

$$L(\boldsymbol{x}_i, y_i) = \max(0, -y_i s_i)$$

Logistic regression (binary classification)

$$s_i = \boldsymbol{w}^T \boldsymbol{x}_i + b$$

- Log-loss when $y \in \{0, 1\}$

$$\hat{y}_i = p(y = 1 | \boldsymbol{x} = \boldsymbol{x}_i) = \frac{1}{1 + e^{-s_i}}$$

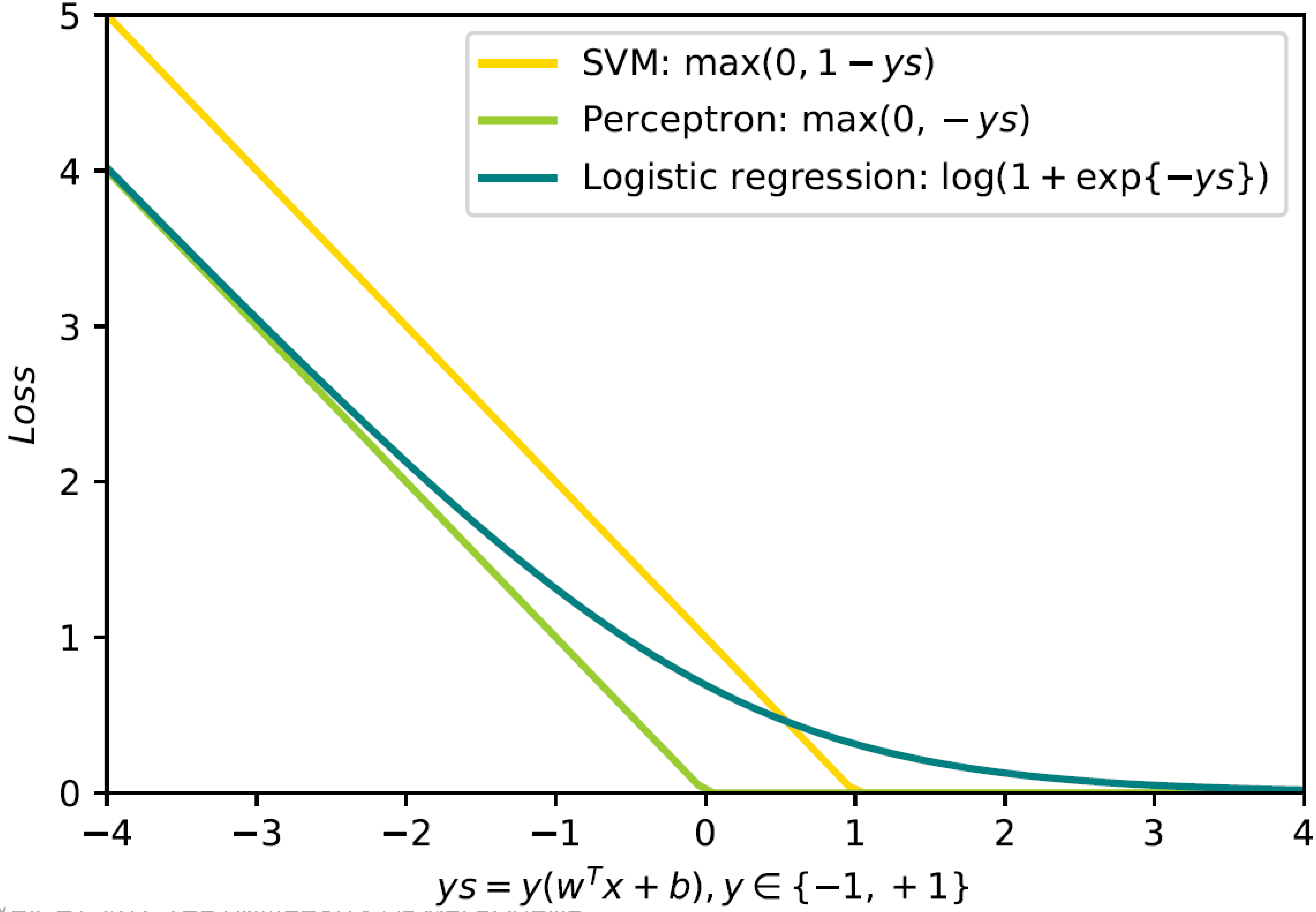
$$L(\boldsymbol{x}_i, y_i) = -(1 - y_i) \log(1 - \hat{y}_i) - y_i \log \hat{y}_i$$

- Log-loss when $y \in \{-1, +1\}$

$$p(y | \boldsymbol{x} = \boldsymbol{x}_i) = \frac{1}{1 + e^{-y s_i}}$$

$$L(\boldsymbol{x}_i, y_i) = -\log p(y = y_i | \boldsymbol{x} = \boldsymbol{x}_i) = \log(1 + e^{-y_i s_i})$$

Loss function for an example $(\boldsymbol{x}, y)$



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Kernel method

- A kernel function is
  - a similarity function over pairs of raw data points
  - the dot product of a pair of transformed data points

$$K(\boldsymbol{u}, \boldsymbol{v}) = \phi(\boldsymbol{u}) \cdot \phi(\boldsymbol{v})$$

- Could be used for many models:
  - SVM, perceptron, logistic regression, linear regression, etc.
- Kernel SVM is the best known one

Kernel method

- Prove a kernel $K(\boldsymbol{u}, \boldsymbol{v})$ is valid by finding its ϕ function

- $K(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u} \cdot \boldsymbol{v} + 1)^2$ is a valid kernel for 2-d points
- Because
- $K(\boldsymbol{u}, \boldsymbol{v}) = (u_1 v_1 + u_2 v_2 + 1)^2 = u_1^2 v_1^2 + u_2^2 v_2^2 + 2u_1 v_1 u_2 v_2 + 2u_1 v_1 + 2u_2 v_2 + 1$
- Let $\phi(\boldsymbol{x}) = \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2} x_1 x_2 & \sqrt{2} x_1 & \sqrt{2} x_2 & 1 \end{bmatrix}$
- Then $K(\boldsymbol{u}, \boldsymbol{v}) = \phi(\boldsymbol{u}) \cdot \phi(\boldsymbol{v})$

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