CSC 561: Neural Networks and Deep Learning

Loss, Overfitting, Model Selection

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Spring 2024

THINK BIG WE DO℠

Loss functions

The “supervised learning” problem

- Finding a **hypothesis** (classifier/regressor) that best approximates a target function $f(\mathbf{x})$
  - the target function maps inputs $\mathbf{x}$ to outputs y from a data-generating distribution P

for $h_w \in \mathscr{H}$ and $\forall (x_i, y_i) \sim P$, we want $h_w(\mathbf{x_i}) \approx f(\mathbf{x_i})$

Machine Learning algorithms use **search and optimization methods for finding** h_w

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Empirical risk minimization

- **True risk** (a.k.a. expected loss, cost function)

$$J^*(\mathbf{w}) = \mathbb{E}\left[l\left(h_w, \mathbf{x_i}, y_i\right)\right]_{(\mathbf{x_i}, y_i)\sim P}$$

  - where l is the **per-example loss** (“error”) between the predicted output $h_w(\mathbf{x_i})$ and the target output y_i

Note that the expectation is taken across the data-generating distribution P rather than over a finite training set.

Empirical risk minimization

- **Empirical risk**
  - we can't solve the true risk directly as we do not know P but only have a training set $\mathcal{D}$ of samples

$$\mathbb{E}\left[l\left(h_w, \mathbf{x_i}, y_i\right)\right]_{(\mathbf{x_i}, y_i)\sim\mathcal{D}} = \frac{1}{n}\sum_{i=1}^{n} l\left(h_w, x_i, y_i\right) = J(\mathbf{w})$$

> Rather than minimizing the **true risk** directly, we optimize the **empirical risk** hoping that the **true loss** decreases significantly as well.

Empirical risk minimization

- The goal of a machine learning algorithm (supervised learning) is to reduce the **true risk**
  - as the true distribution P is unknown we can minimize the empirical risk instead
- The training process based on minimizing the **empirical risk** is known as **empirical risk minimization**

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} J(\mathbf{w})$$

0/1 loss

$$l_{0/1}(h_w, \mathbf{x_i}, y_i) = I\left(h_w(\mathbf{x_i}) \neq y_i\right)$$

indicator function

Prediction	Target
5	5
1	9
2	2
7	7
8	0
0	0
0	8
3	3
6	6
4	4

Empirical risk?

Practice

X0	X1	X2	Y
1	0	0	-1
1	1	0	+1
1	1	1	+1
1	0	1	+1

$$h_w(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x})$$

$$\sigma(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases}$$

zero-one loss for $\mathbf{w}_a = [0,0,0]^T$?

zero-one loss for $\mathbf{w}_b = [0,1,0]^T$?

zero one loss for $\mathbf{w}_c = [-1,2,2]^T$?

Squared loss

$$l_{sq}(h_w, \mathbf{x_i}, y_i) = \left(h_w(\mathbf{x_i}) - y_i\right)^2$$

penalizes big mistakes

Prediction	Target
1.2	1.4
2.3	2.3
1.1	1.2
3.4	4.1
2.3	2.5
1.1	1.1
2.5	2.6
3.1	3.2
1.7	1.8
2.3	2.3

Empirical risk?

Absolute loss

$$l_{abs}(h_w, \mathbf{x_i}, y_i) = \left| h_w(\mathbf{x_i}) - y_i \right|$$

Prediction	Target
1.2	1.4
2.3	2.3
1.1	1.2
3.4	4.1
2.3	2.5
1.1	1.1
2.5	2.6
3.1	3.2
1.7	1.8
2.3	2.3

Empirical risk?

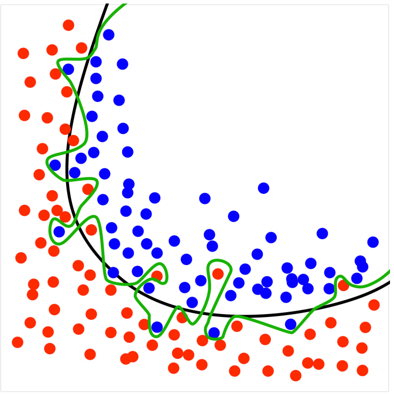
Remarks

- Empirical risk minimization is prone to **overfitting**
  - high-capacity models can simply memorize the training set
  - can introduce regularization to improve generalization
- Modern machine learning is based on **gradient descent**
  - requires loss functions to be differentiable (e.g., can't use 0/1 loss)
- In the context of deep learning, we must go beyond pure empirical risk minimization
  - the quantity that we actually optimize may differ from the quantity we truly want to optimize
  - e.g. SGD does not directly optimize the empirical risk, rather a loss function that approximates it

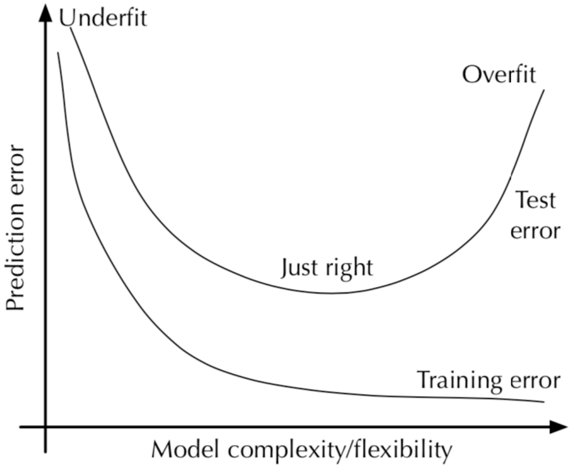
Overfitting

Overfitting

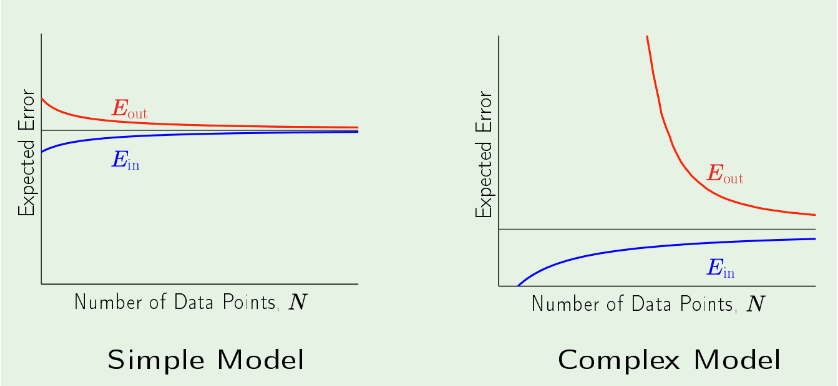
- Learning a model that "knows" the training data very well but does not generalize



Model complexity



Number of data instances



https://work.caltech.edu/lectures.html

Overfitting

- Reasons
  - ✓ model is too complex
  - ✓ model is fitting noise present in the training data
  - ✓ training data is not a representative sample of the distribution
- How to prevent?
  - ✓ use more training data
  - ✓ use fewer features
  - ✓ regularize your model

Generalization

- We can use a ML method to calculate:

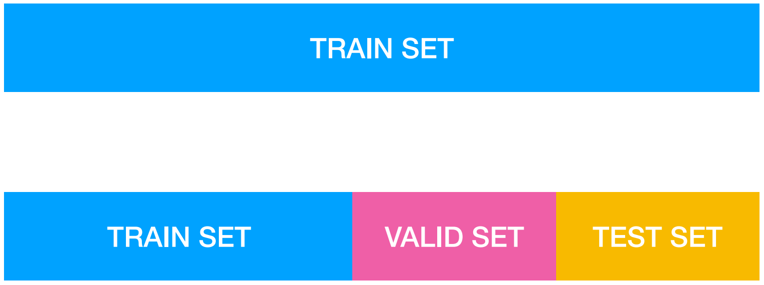
$$\mathbf{w}^* = \arg\min_{\mathbf{w}} J(\mathbf{w})$$

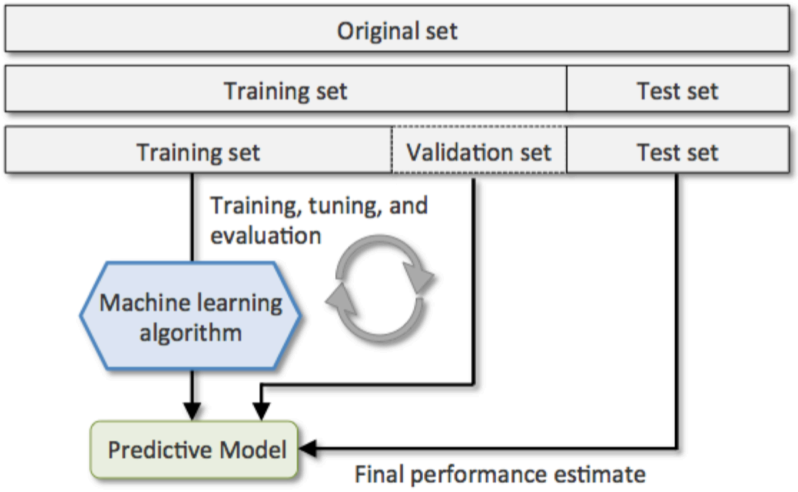
- Problem: it may overfit the training data
  - ✓ we want better generalization
- Solution: split your data in train, validation, test
  - ✓ use train and validation to select the best hypothesis
  - ✓ use test for final evaluation and report

Model selection

Train and test

Train, validation, and test





from INFO-4604: Applied Machine Learning, Fall 2017, Michael Paul, Univ. of Colorado

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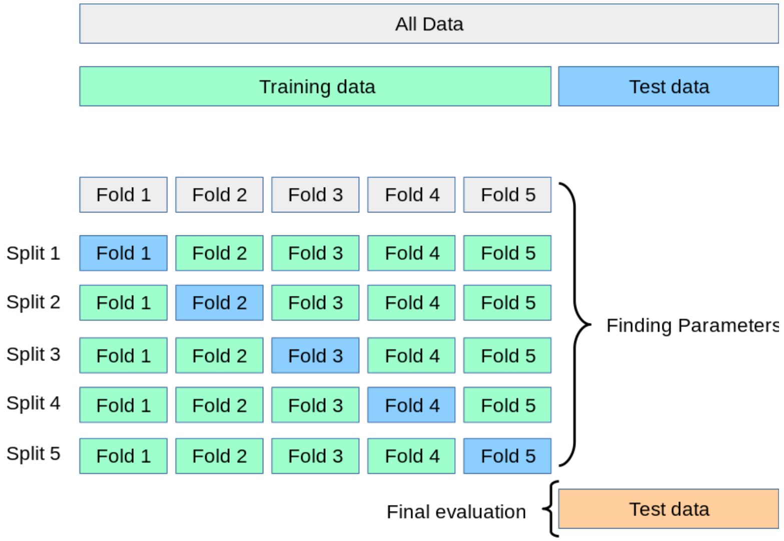
k-fold cross validation



https://scikit-learn.org/stable/modules/cross_validation.html

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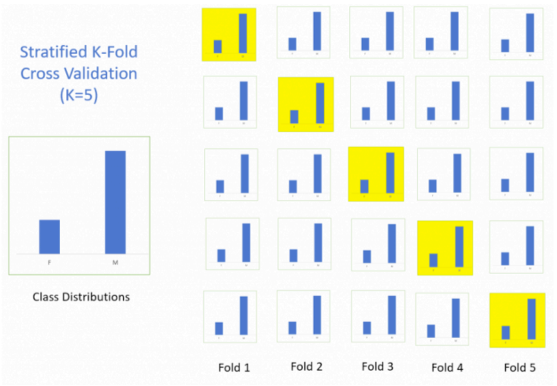
Stratified cross validation

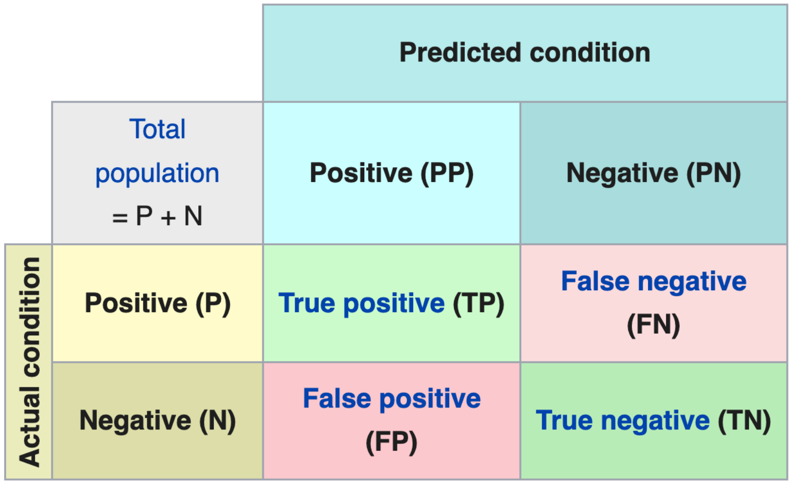


Stratified cross validation aims at having the same class distribution within each fold

https://towardsdatascience.com/cross-validation-explained-evaluating-estimator-performance-e51e5430ff85

Evaluation

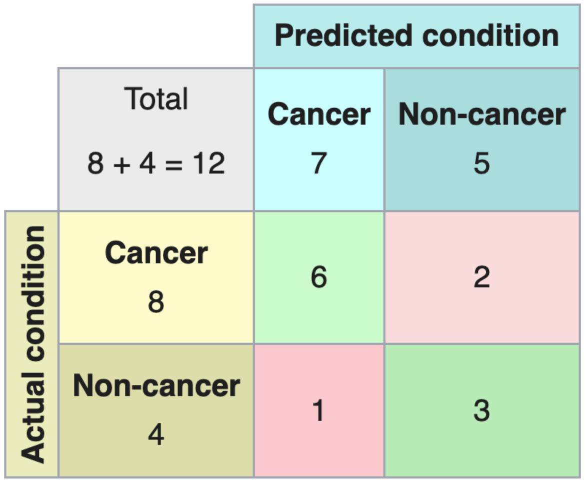
Confusion matrix (2 classes)



		Predicted condition	
	Total population = P + N	Positive (PP)	Negative (PN)
Actual condition	Positive (P)	True positive (TP)	False negative (FN)
	Negative (N)	False positive (FP)	True negative (TN)

https://en.wikipedia.org/wiki/Confusion_matrix

Confusion matrix (example)



		Predicted condition	
	Total 8 + 4 = 12	Cancer 7	Non-cancer 5
Actual condition	Cancer 8	6	2
	Non-cancer 4	1	3

https://en.wikipedia.org/wiki/Confusion_matrix

Evaluation metrics (2 classes)

accuracy (ACC)

$$\mathrm{ACC} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{P} + \mathrm{N}} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}}$$

F1 score

is the harmonic mean of precision and sensitivity

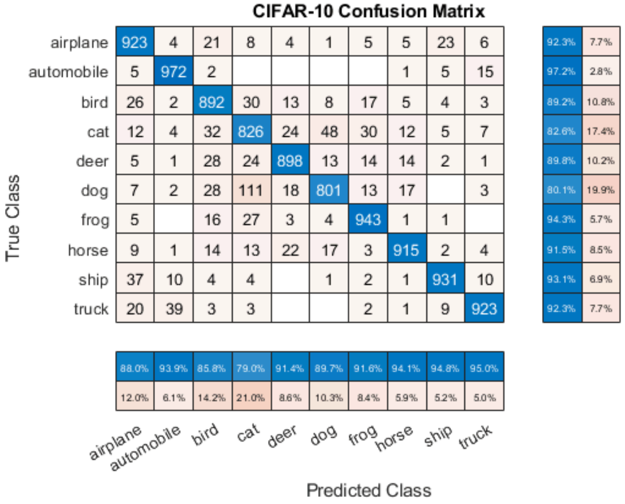
$$\mathrm{F}_1 = 2 \cdot \frac{\mathrm{PPV} \cdot \mathrm{TPR}}{\mathrm{PPV} + \mathrm{TPR}} = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

Matthews correlation coefficient (MCC)

$$\mathrm{MCC} = \frac{\mathrm{TP} \times \mathrm{TN} - \mathrm{FP} \times \mathrm{FN}}{\sqrt{(\mathrm{TP} + \mathrm{FP})(\mathrm{TP} + \mathrm{FN})(\mathrm{TN} + \mathrm{FP})(\mathrm{TN} + \mathrm{FN})}}$$

https://en.wikipedia.org/wiki/Confusion_matrix

Confusion matrix (example >2 classes)



CIFAR-10 Confusion Matrix

	airplane	automobile	bird	cat	deer	dog	frog	horse	ship	truck		
airplane	923	4	21	8	4	1	5	5	23	6	92.3%	7.7%
automobile	5	972	2					1	5	15	97.2%	2.8%
bird	26	2	892	30	13	8	17	5	4	3	89.2%	10.8%
cat	12	4	32	826	24	48	30	12	5	7	82.6%	17.4%
deer	5	1	28	24	898	13	14	14	2	1	89.8%	10.2%
dog	7	2	28	111	18	801	13	17		3	80.1%	19.9%
frog	5		16	27	3	4	943	1	1		94.3%	5.7%
horse	9	1	14	13	22	17	3	915	2	4	91.5%	8.5%
ship	37	10	4	4		1	2	1	931	10	93.1%	6.9%
truck	20	39	3	3			2	1	9	923	92.3%	7.7%
	88.0%	93.9%	85.8%	79.0%	91.4%	89.7%	91.6%	94.1%	94.8%	95.0%		
	12.0%	6.1%	14.2%	21.0%	8.6%	10.3%	8.4%	5.9%	5.2%	5.0%		

https://www.mathworks.com/help/deeplearning/ref/confusionchart.html