More Data Mining with Weka

Class 5 – Lesson 1

Simple neural networks

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Lesson 5.1: Simple neural networks

Class 1	**Exploring Weka's interfaces; working with big data**
Class 2	**Discretization and text classification**
Class 3	**Classification rules, association rules, and clustering**
Class 4	**Selecting attributes and counting the cost**
Class 5	**Neural networks, learning curves, and performance optimization**

Lesson 5.1 Simple neural networks

Lesson 5.2 Multilayer Perceptrons

Lesson 5.3 Learning curves

Lesson 5.4 Performance optimization

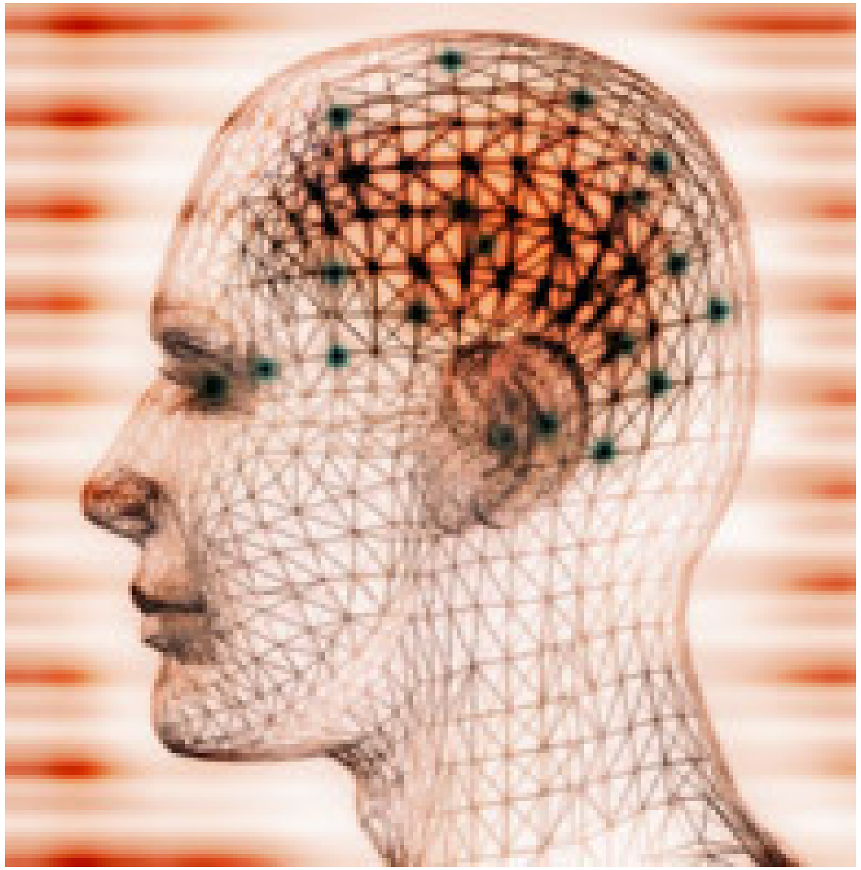
Lesson 5.5 ARFF and XRFF

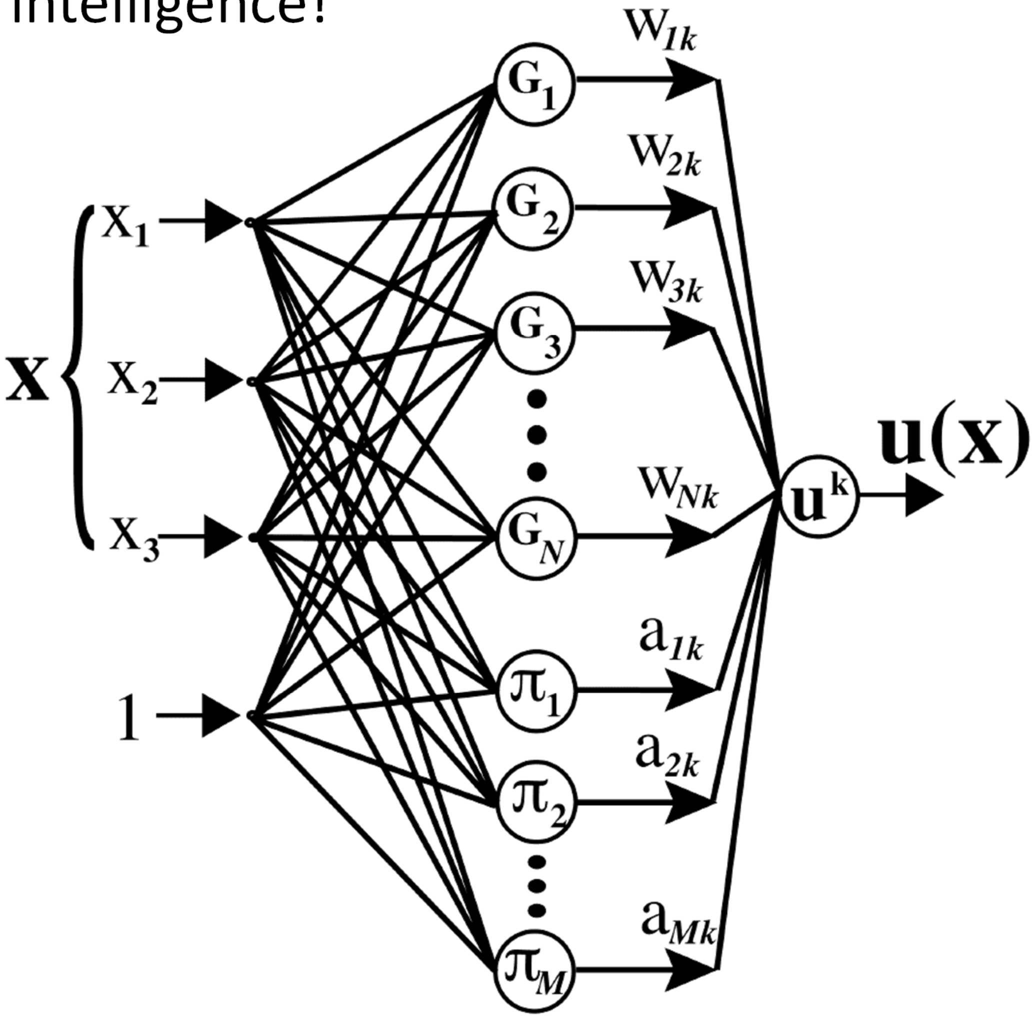
Lesson 5.6 Summary

Lesson 5.1: Simple neural networks

Many people love neural networks (not me)

… the very name is suggestive of … intelligence!

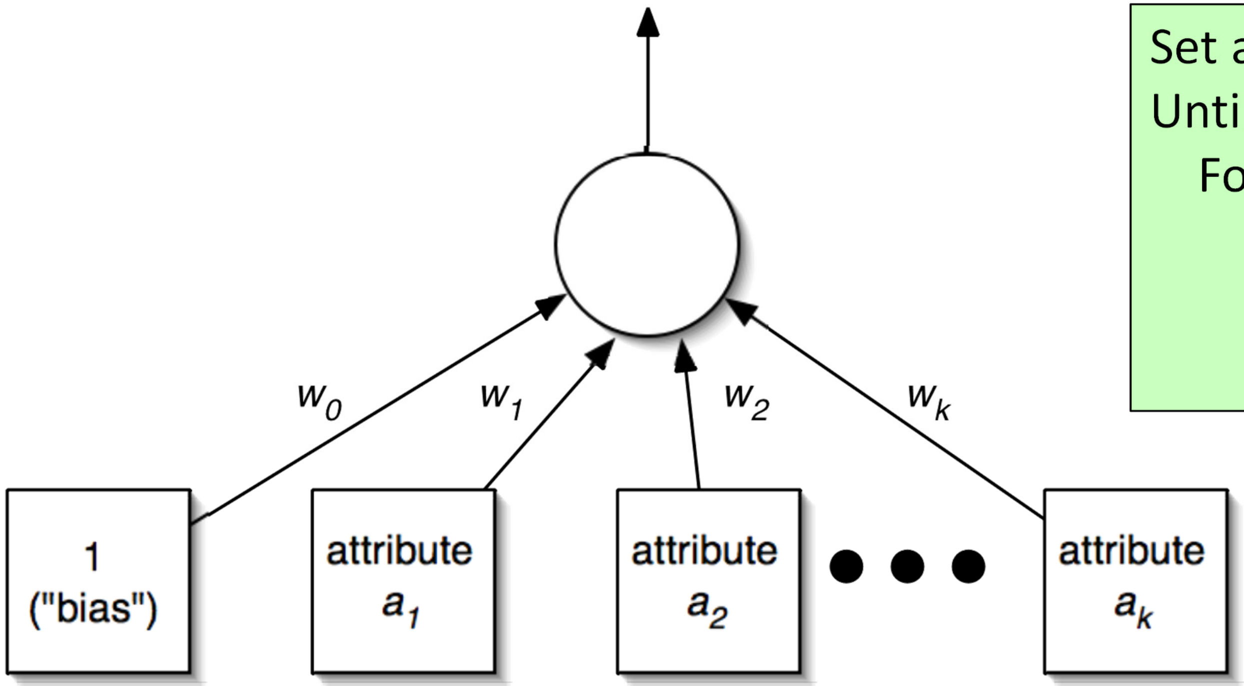




Lesson 5.1: Simple neural networks

Perceptron: simplest form

- Determine the class using a linear combination of attributes
- for test instance **a**, $x = w_0 + w_1 a_1 + w_2 a_2 + \ldots + w_k a_k = \sum_{j=0}^{k} w_j a_j$
- if $x > 0$ then class 1, if $x < 0$ then class 2
  - *Works most naturally with numeric attributes*




```
Set all weights to zero
Until all instances in the training data are classified correctly
    For each instance i in the training data
        If i is classified incorrectly
            If i belongs to the first class add it to the weight vector
            else subtract it from the weight vector
```

Perceptron convergence theorem

- *converges if you cycle repeatedly through the training data*
- *provided the problem is "linearly separable"*

Lesson 5.1: Simple neural networks

Linear decision boundaries

- Recall Support Vector Machines (Data Mining with Weka, lesson 4.5)
  - *also restricted to linear decision boundaries*
  - *but can get more complex boundaries with the "Kernel trick" (not explained)*
- Perceptron can use the same trick to get non-linear boundaries

Voted perceptron (in Weka)

- Store all weight vectors and let them vote on test examples
  - *weight them according to their "survival" time*
- Claimed to have many of the advantages of Support Vector Machines
- … faster, simpler, and nearly as good

Lesson 5.1: Simple neural networks

How good is VotedPerceptron?

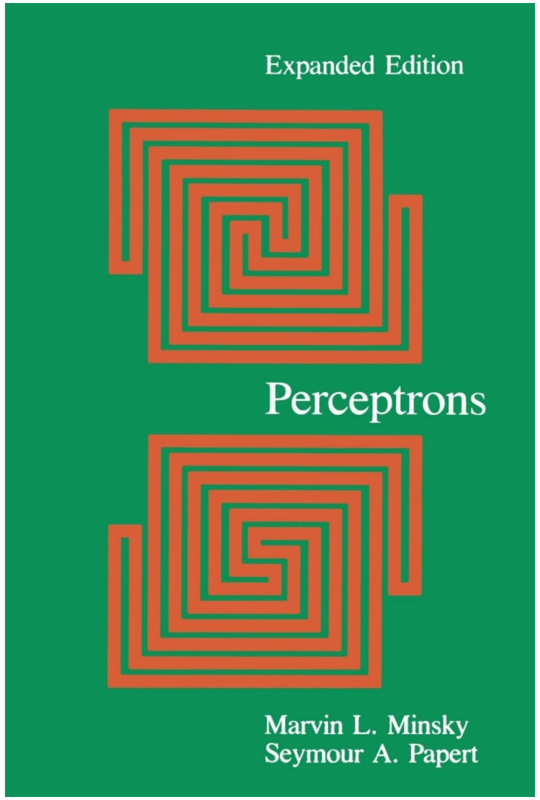
	VotedPerceptron	*SMO*
Ionosphere dataset ionosphere.arff	86%	89%
German credit dataset credit-g.arff	70%	75%
Breast cancer dataset breast-cancer.arff	71%	70%
Diabetes dataset diabetes.arff	67%	77%

Is it faster? … yes

Lesson 5.1: Simple neural networks

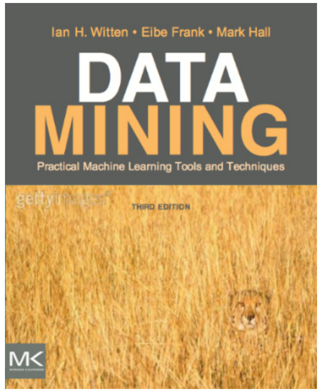
History of the Perceptron

- 1957: Basic perceptron algorithm
  - *Derived from theories about how the brain works*
  - *"A perceiving and recognizing automaton"*
  - *Rosenblatt "Principles of neurodynamics: Perceptrons and the theory of brain mechanisms"*
- 1970: Suddenly went out of fashion
  - *Minsky and Papert "Perceptrons"*
- 1986: Returned, rebranded "connectionism"
  - *Rumelhart and McClelland "Parallel distributed processing"*
  - *Some claim that artificial neural networks mirror brain function*
- Multilayer perceptrons
  - *Nonlinear decision boundaries*
  - *Backpropagation algorithm*



Lesson 5.1: Simple neural networks

- Basic Perceptron algorithm: linear decision boundary
  - Like classification-by-regression
  - Works with numeric attributes
  - Iterative algorithm, order dependent
- My MSc thesis (1971) describes a simple improvement!
  - Still not impressed, sorry
- Modern improvements (1999):
  - get more complex boundaries using the "Kernel trick"
  - more sophisticated strategy with multiple weight vectors and voting



Course text

- Section 4.6 *Linear classification using the Perceptron*
- Section 6.4 *Kernel Perceptron*

More Data Mining with Weka

Class 5 – Lesson 2

Multilayer Perceptrons

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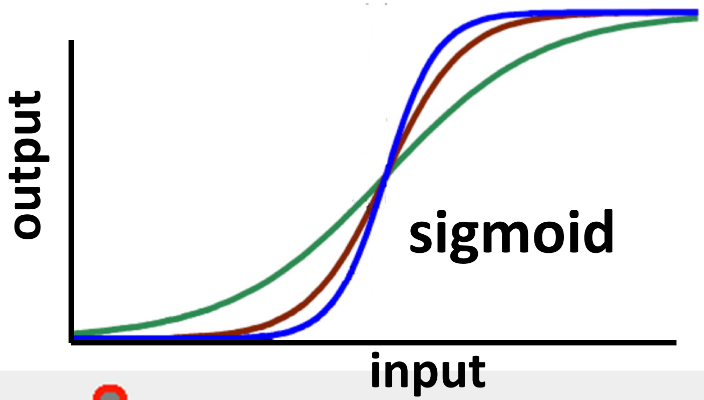
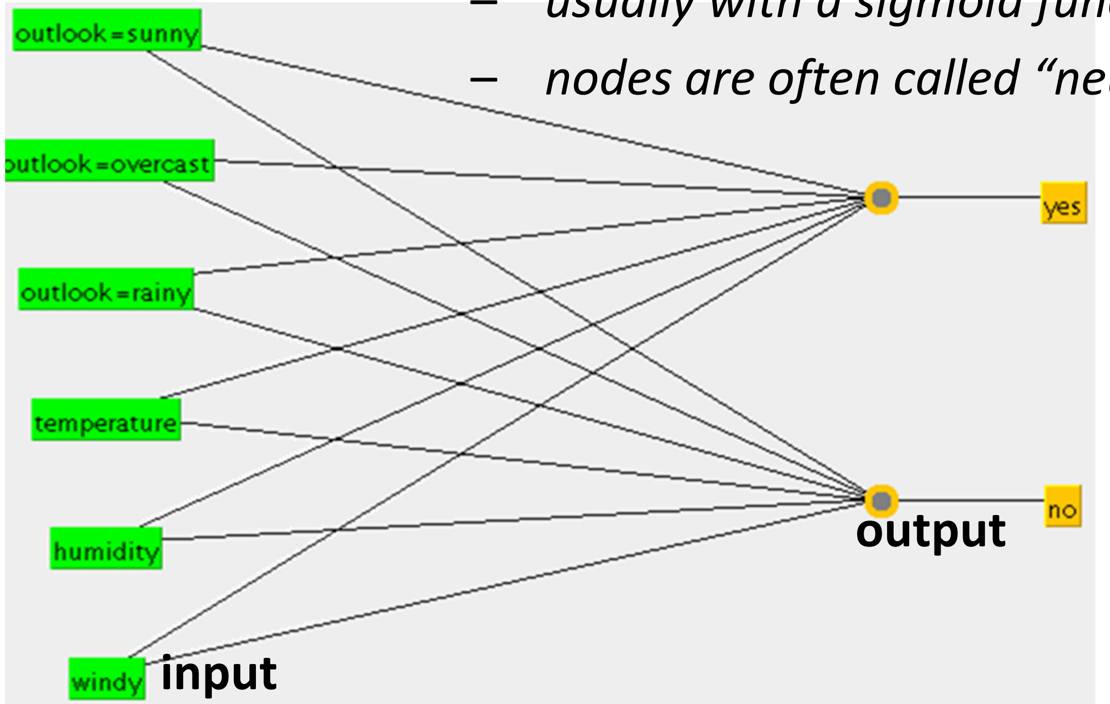
Lesson 5.2: Multilayer Perceptrons

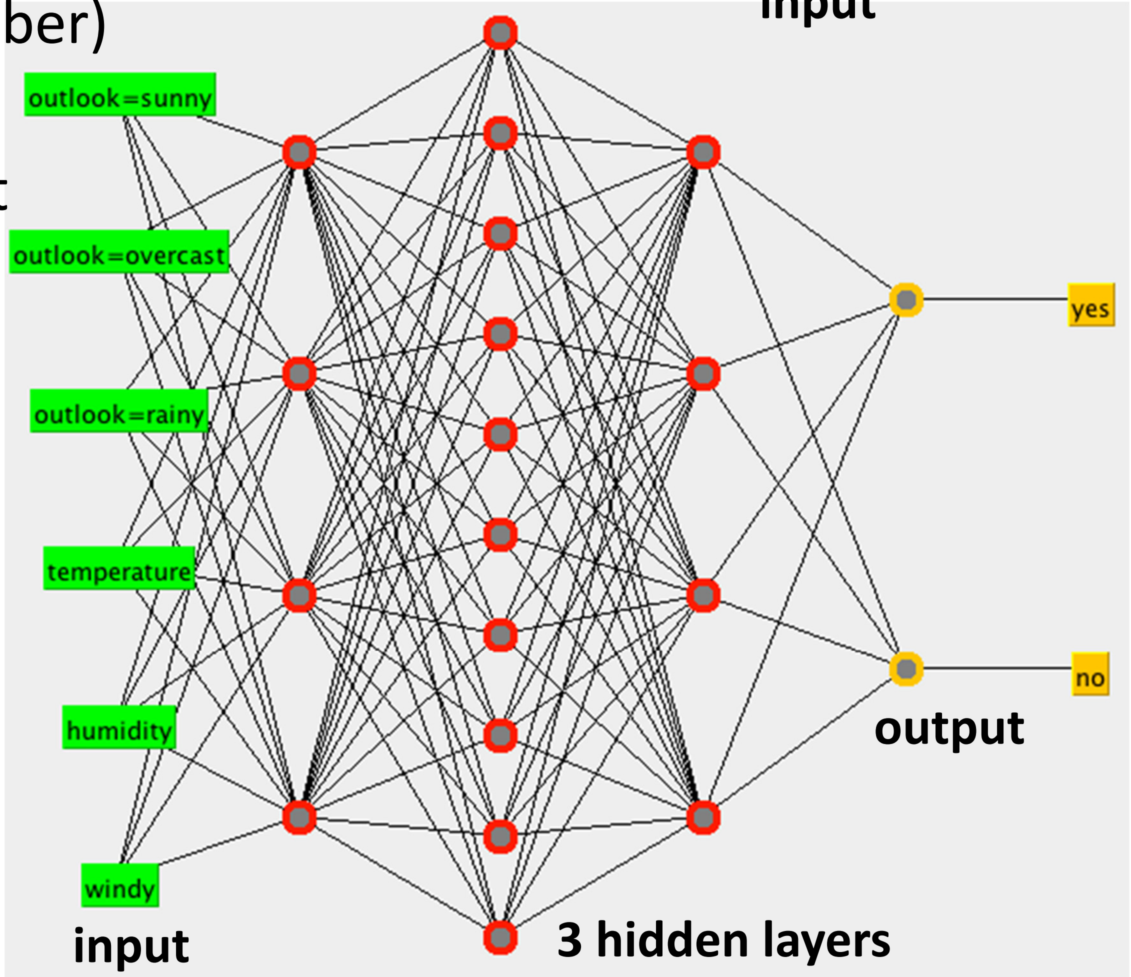
Lesson 5.2: Multilayer Perceptrons



Network of perceptrons

- Input layer, hidden layer(s), and output layer
- Each connection has a weight (a number)
- Each node performs a weighted sum of its inputs and thresholds the result
  - *usually with a sigmoid function*
  - *nodes are often called "neurons"*





Lesson 5.2: Multilayer Perceptrons

How many layers, how many nodes in each?

- Input layer: one for each attribute (attributes are numeric, or binary)
- Output layer: one for each class (or just one if the class is numeric)
- How many hidden layers? — Big Question #1
- Zero hidden layers:
  - *standard Perceptron algorithm*
  - *suitable if data is linearly separable*
- One hidden layer:
  - *suitable for a single convex region of the decision space*
- Two hidden layers:
  - *can generate arbitrary decision boundaries*
- How big are they? — Big Question #2
  - *usually chosen somewhere between the input and output layers*
  - *common heuristic: mean value of input and output layers (Weka's default)*

Lesson 5.2: Multilayer Perceptrons

What are the weights?

- They're learned from the training set
- Iteratively minimize the error using steepest descent
- Gradient is determined using the "backpropagation" algorithm
- Change in weight computed by multiplying the gradient by the "learning rate" and adding the previous change in weight multiplied by the "momentum":

$$W_{next} = W + \Delta W$$
$$\Delta W = -\text{learning\_rate} \times \text{gradient} \; + \; \text{momentum} \times \Delta W_{previous}$$

Can get excellent results

- Often involves (much) experimentation
  - *number and size of hidden layers*
  - *value of learning rate and momentum*

Lesson 5.2: Multilayer Perceptrons

MultilayerPerceptron performance

- Numeric weather data 79%!
- (J48, NaiveBayes both 64%, SMO 57%, IBk 79%)
- On real problems does quite well – but slow

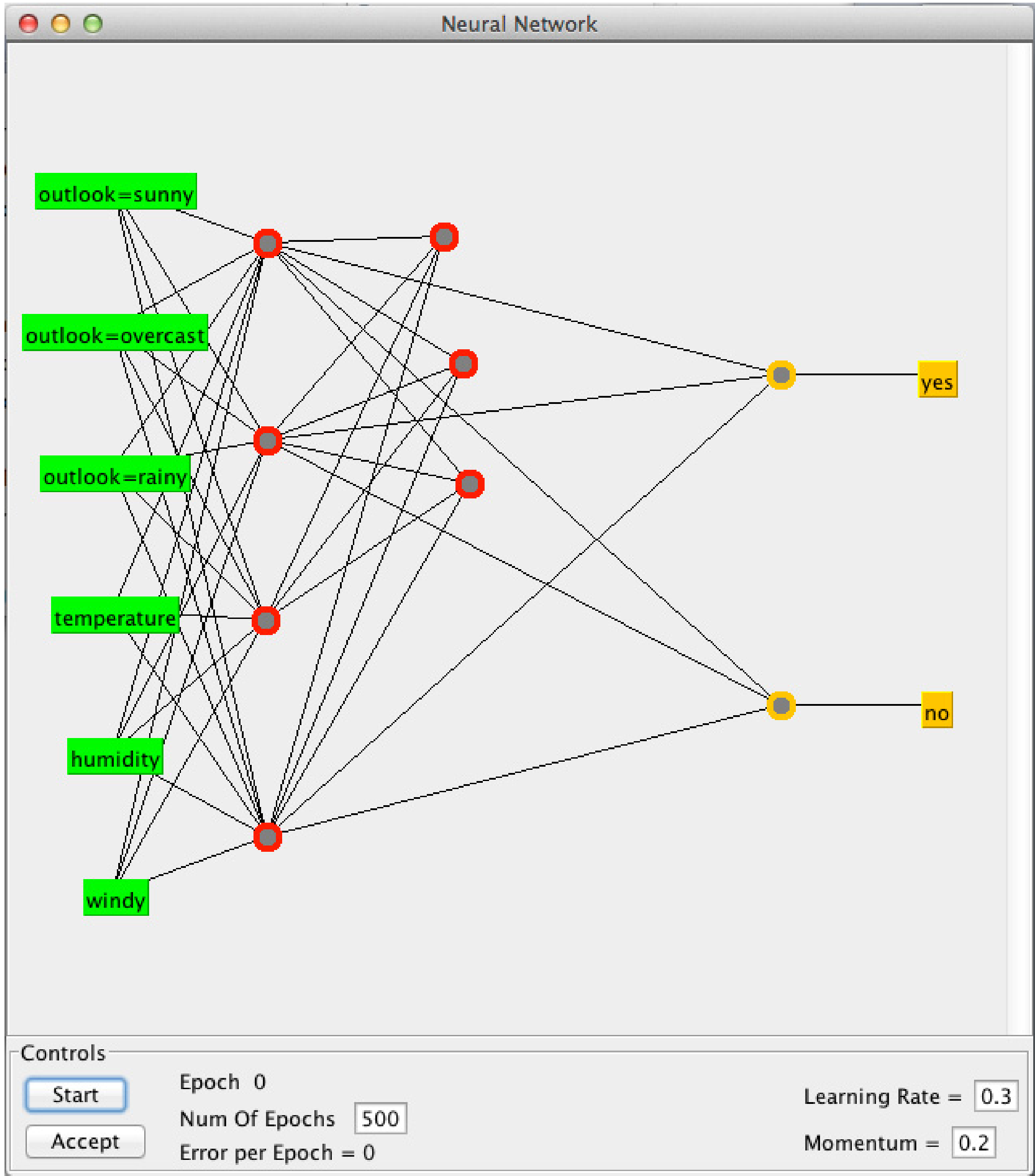
Parameters

- hiddenLayers: set GUI to *true* and try 5, 10, 20
- learningRate, momentum
- makes multiple passes (“epochs”) through the data
- training continues until
  - *error on the validation set consistently increases*
  - *or training time is exceeded*

Lesson 5.2: Multilayer Perceptrons

Create your own network structure!

- Selecting nodes
  - *click to select*
  - *right-click in empty space to deselect*
- Creating/deleting nodes
  - *click in empty space to create*
  - *right-click (with no node selected) to delete*
- Creating/deleting connections
  - *with a node selected, click on another to connect to it*
  - *… and another, and another*
  - *right-click to delete connection*
- Can set parameters here too



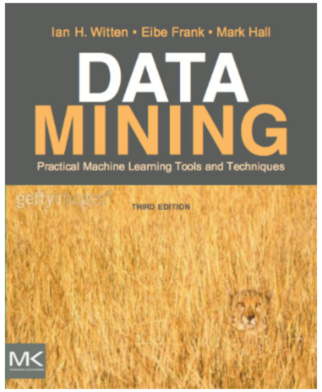
Lesson 5.2: Multilayer Perceptrons

Are they any good?

- Experimenter with 6 datasets
  - *Iris, breast-cancer, credit-g, diabetes, glass, ionosphere*
- 9 algorithms
  - *MultilayerPerceptron, ZeroR, OneR, J48, NaiveBayes, IBk, SMO, AdaBoostM1, VotedPerceptron*
- MultilayerPerceptron wins on 2 datasets
- Other wins:
  - *SMO on 2 datasets*
  - *J48 on 1 dataset*
  - *IBk on 1 dataset*
- But … 10–2000 times slower than other methods

Lesson 5.2: Multilayer Perceptrons

- Multilayer Perceptrons implement arbitrary decision boundaries
  - given two (or more) hidden layers, that are large enough
  - and are trained properly
- Training by backpropagation
  - iterative algorithm based on gradient descent
- In practice??
  - Quite good performance, but extremely slow
  - Still not impressed, sorry
  - Might be a lot more impressive on more complex datasets



Course text

- Section 4.6 *Linear classification using the Perceptron*
- Section 6.4 *Kernel Perceptron*

More Data Mining with Weka

Class 5 – Lesson 3

Learning curves

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Lesson 5.3: Learning curves

Class 1 **Exploring Weka's interfaces; working with big data**

Class 2 **Discretization and text classification**

Class 3 **Classification rules, association rules, and clustering**

Class 4 **Selecting attributes and counting the cost**

Class 5 **Neural networks, learning curves, and performance optimization**

Lesson 5.1 Simple neural networks

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Lesson 5.3 Learning curves

Lesson 5.4 Performance optimization

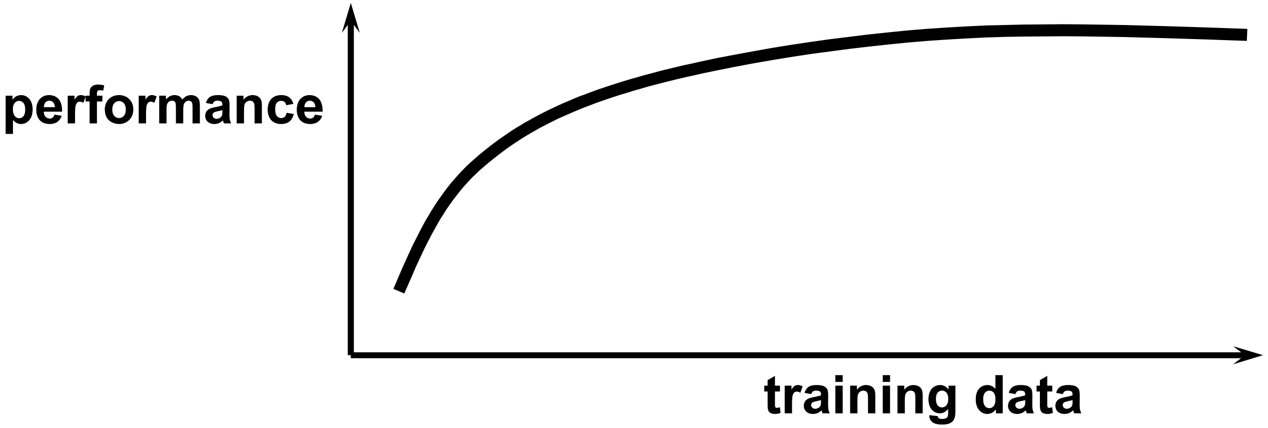
Lesson 5.5 ARFF and XRFF

Lesson 5.6 Summary

Lesson 5.3: Learning curves

The advice on evaluation (from "Data Mining with Weka")

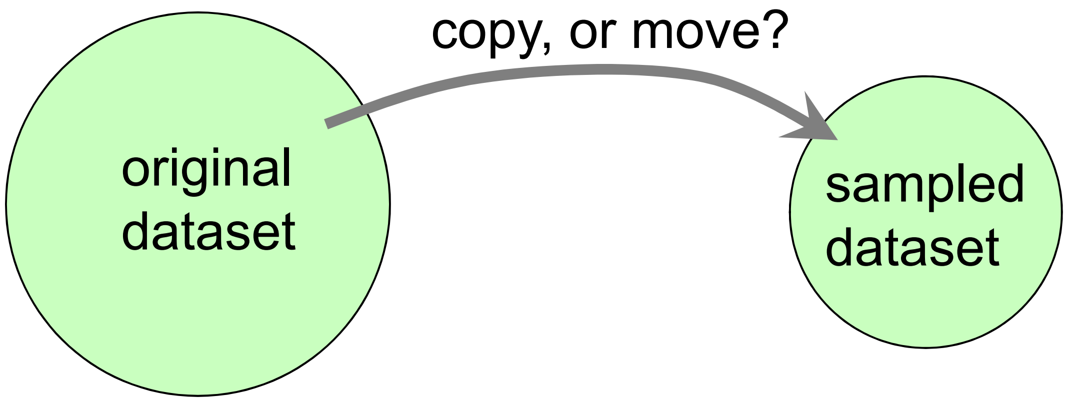
- Large separate test set? … use it
- Lots of data? … use holdout
- Otherwise, use 10-fold cross-validation
  - *and repeat 10 times, as the Experimenter does*
- But … how much is a lot?
- It depends
  - *on number of classes*
  - *number of attributes*
  - *structure of the domain*
  - *kind of model …*
- Learning curves



Lesson 5.3: Learning curves

Plotting a learning curve

- Resample filter:
  replacement vs. no replacement

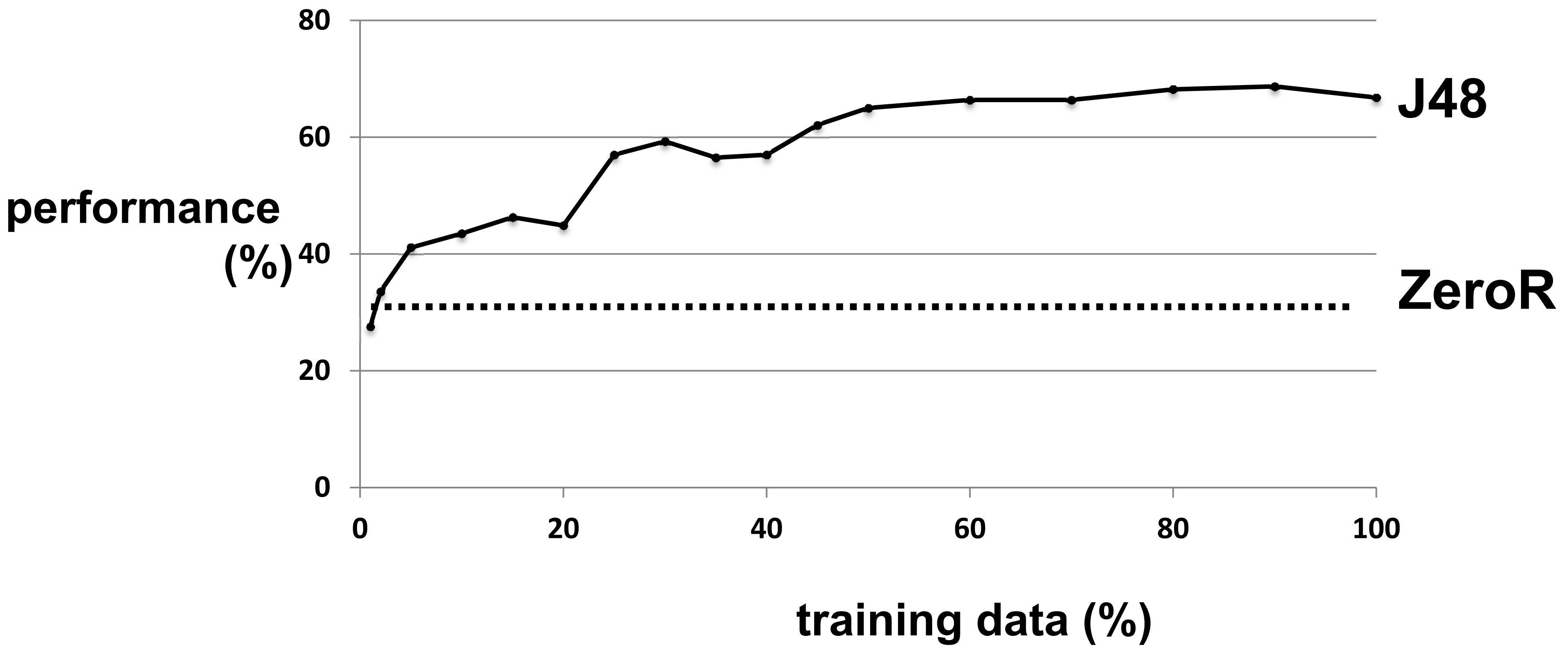


- Sample training set but not test set
- Meta > FilteredClassifier
  Resample (no replacement), 50% sample, J48, 10-fold cross-validation
- Glass dataset (214 instances, 6 classes)

Lesson 5.3: Learning curves

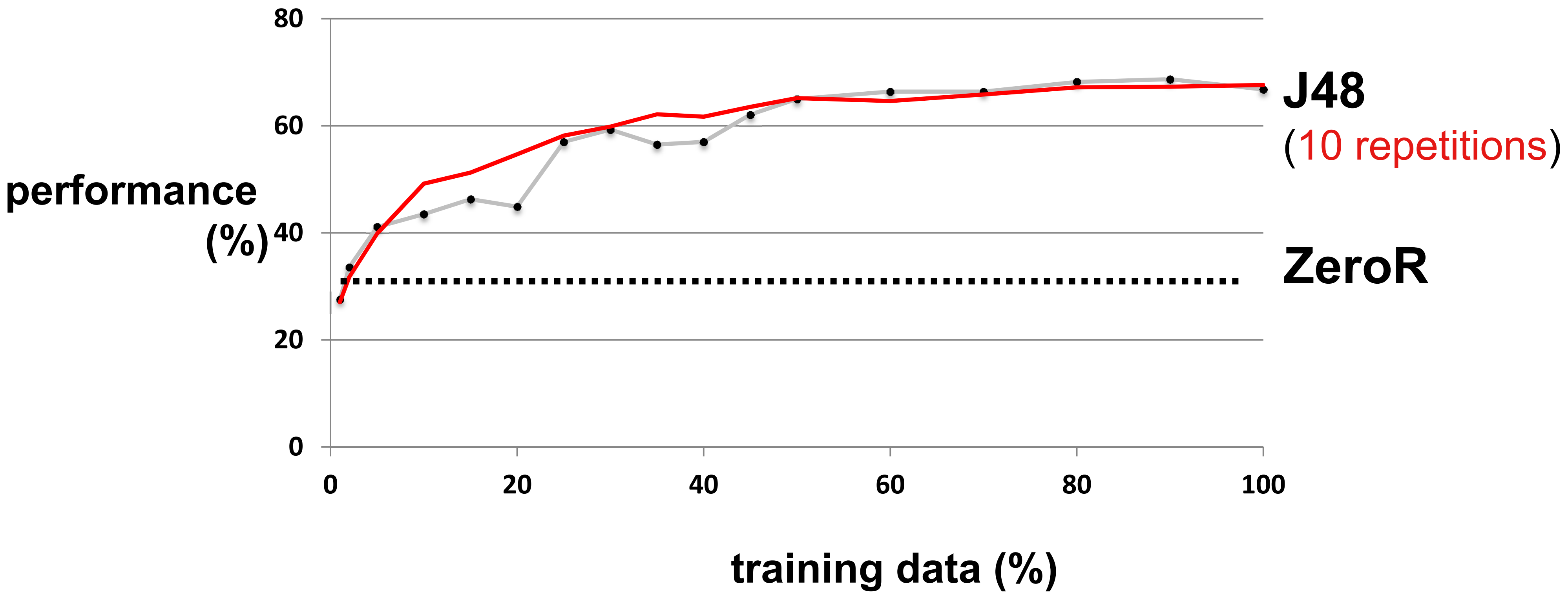
An empirical learning curve

100%	66.8%
90%	68.7%
80%	68.2%
70%	66.4%
60%	66.4%
50%	65.0%
45%	62.1%
40%	57.0%
35%	56.5%
30%	59.3%
25%	57.0%
20%	44.9%
10%	43.5%
5%	41.1%
2%	33.6%
1%	27.6%



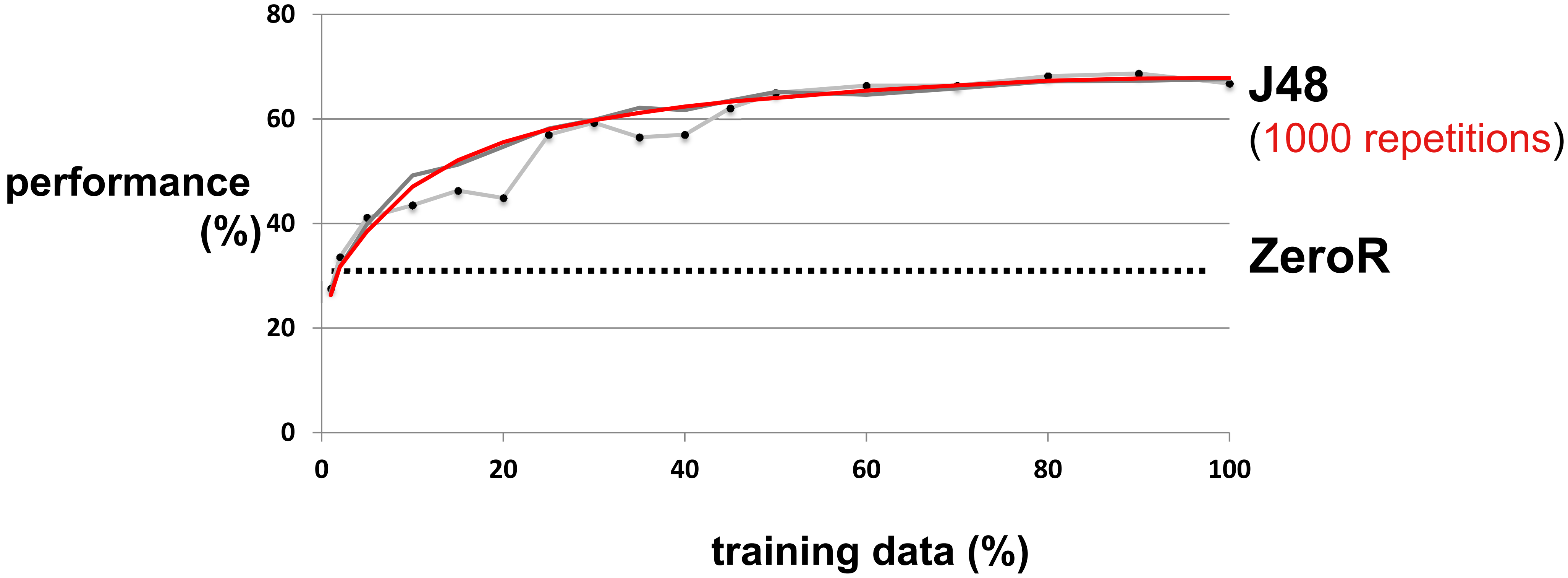
Lesson 5.3: Learning curves

An empirical learning curve



Lesson 5.3: Learning curves

An empirical learning curve



Lesson 5.3: Learning curves

- How much data is enough?
- Hard to say!
- Plot learning curve?
- Resampling (with/without replacement)
- … but don't sample the test set!
- meta > FilteredClassifier
- Note:

  performance figure is only an estimate

More Data Mining with Weka

Class 5 – Lesson 4

Meta-learners for performance optimization

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Lesson 5.4: Meta-learners for performance optimization

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Lesson 5.2 Multilayer Perceptrons

Lesson 5.3 Learning curves

Lesson 5.4 Performance optimization

Lesson 5.5 ARFF and XRFF

Lesson 5.6 Summary

Lesson 5.4: Meta-learners for performance optimization

"Wrapper" meta-learners in Weka

Recall AttributeSelectedClassifier with WrapperSubsetEval
- *selects an attribute subset based on how well a classifier performs*
- *uses cross-validation to assess performance*

1. **CVParameterSelection**: selects best value for a parameter
   - *optimizes performance, using cross-validation*
   - *optimizes accuracy (classification) or root mean-squared error (regression)*
2. **GridSearch**
   - *optimizes two parameters by searching a 2D grid*
3. **ThresholdSelector**
   - *selects a probability threshold on the classifier's output*
   - *can optimize accuracy, true positive rate, precision, recall, F-measure*

Lesson 5.4: Meta-learners for performance optimization

Try CVParameterSelection

- J48 has two parameters, confidenceFactor C and minNumObj M
  - *in Data Mining with Weka, I advised not to play with confidenceFactor*
- Load diabetes.arff, select J48: 73.8%
- CVParameterSelection with J48
- confidenceFactor from 0.1 to 1.0 in 10 steps: C 0.1 1 10
  - *check More button*
  - *use* C 0.1 0.9 9
- Achieves 73.4% with C = 0.1 ☹
- minNumObj from 1 to 10 in 10 steps
  - *add* M 1 10 10 *(first)*
- Achieves 74.3% with C = 0.2 and M = 10; simpler tree
  - *takes a while!*

Lesson 5.4: Meta-learners for performance optimization

GridSearch

- CVParameterSelection with multiple parameters
  - *first one, then the other*
- GridSearch optimizes two parameters together
- Can explore best parameter combinations for a filter and classifier
- Can optimize accuracy (classification) or various measures (regression)
- Very flexible but fairly complicated to set up
- Take a quick look …

Lesson 5.4: Meta-learners for performance optimization

ThresholdSelector

In Lesson 4.6 (cost-sensitive classification), we looked at probability thresholds

- Credit dataset credit-g.arff, NaiveBayes, 75.4%
- Output predictions
- Weka chooses *good* if Pr[good] > Pr[bad], i.e. threshold = 0.5:
  - predicts 756 *good*, with 151 mistakes
  - 244 *bad*, with 95 mistakes

a	b		<-- classified as
605	95	|	a = good
151	149	|	b = bad

- Can optimize threshold with ThresholdSelector
  - *though unlikely to do better*

	actual	predicted	p_{good}	p_{bad}
0	good	good	0.999	0.001
50	good	good	0.991	0.009
100	good	good	0.983	0.017
150	good	good	0.975	0.025
200	good	good	0.965	0.035
250	bad	good	0.951	0.049
300	bad	good	0.934	0.066
350	good	good	0.917	0.083
400	good	good	0.896	0.104
450	good	good	0.873	0.127
500	good	good	0.836	0.164
550	good	good	0.776	0.224
600	bad	good	0.715	0.285
650	good	good	0.663	0.337
700	good	good	0.587	0.413
750	bad	good	0.508	0.492
800	good	bad	0.416	0.584
850	bad	bad	0.297	0.703
900	good	bad	0.184	0.816
950	bad	bad	0.04	0.96

Lesson 5.4: Meta-learners for performance optimization

Try ThresholdSelector

- Credit dataset credit-g.arff, NaiveBayes 75.4%
- ThresholdSelector, NaiveBayes, optimize Accuracy 75.4%
  - *NB designatedClass should be the **first** class value*
- But you can optimize other things!

FMEASURE
✓ ACCURACY
TRUE_POS
TRUE_NEG
TP_RATE
PRECISION
RECALL

- Confusion matrix

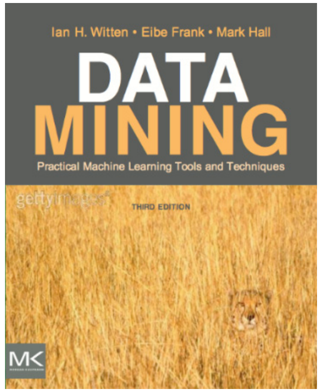
a	b	<-- classified as
TP	FN	| a = good
FP	TN	| b = bad

- Precision $\dfrac{\text{number correctly classified as } good}{\text{total number classified as } good} = \dfrac{TP}{TP+FP}$
- Recall $\dfrac{\text{number correctly classified as } good}{\text{actual number of } good \text{ instances}} = \dfrac{TP}{TP+FN}$
- F-measure $\dfrac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$

Lesson 5.4: Meta-learners for performance optimization

- Don’t optimize parameters manually
  - you’ll overfit!
- Wrapper method uses internal cross-validation to optimize

1. CVParameterSelection — optimize parameters individually
2. GridSearch — optimize two parameters together
3. ThresholdSelection — select a probability threshold



Course text

- Section 11.5 *Optimizing performance*
- Section 5.7 *Recall–Precision curves*

More Data Mining with Weka

Class 5 – Lesson 5

ARFF and XRFF

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Lesson 5.5: ARFF and XRFF

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- **Lesson 5.1 Simple neural networks**
- **Lesson 5.2 Multilayer Perceptrons**
- **Lesson 5.3 Learning curves**
- **Lesson 5.4 Performance optimization**
- **Lesson 5.5 ARFF and XRFF**
- **Lesson 5.6 Summary**

Lesson 5.5: ARFF and XRFF

ARFF format revisited

@relation

@attribute

- *nominal, numeric (integer or real), string*

@data

data lines (“?” for a missing value)

% comment lines

```
@relation weather

@attribute outlook {sunny, overcast, rainy}
@attribute temperature numeric
@attribute humidity numeric
@attribute windy {TRUE, FALSE}
@attribute play {yes, no}

@data
sunny, 85, 85, FALSE, no
sunny, 80, 90, TRUE, no
…
rainy, 71, 91, TRUE, no
```

Lesson 5.5: ARFF and XRFF

```
@relation weather.symbolic

@attribute outlook {sunny, overc
@attribute temperature {hot, mi
@attribute humidity {high, norm
@attribute windy {TRUE, FALSE}
@attribute play {yes, no}

@data
```

ARFF format: more

```
sunny, hot, high, FALSE, no
sunny, hot, high, TRUE, no
overcast, hot, high, FALSE, yes
rainy, mild, high, FALSE, yes
rainy, cool, normal, FALSE, yes
rainy, cool, normal, TRUE, no
overcast, cool, normal, TRUE, yes
```

```
{3 FALSE, 4 no}
{4 no}
{0 overcast, 3 FALSE}
{0 rainy, 1 mild, 3 FALSE}
{0 rainy, 1 cool, 2 normal, 3 FALSE}
{0 rainy, 1 cool, 2 normal, 4 no}
{0 overcast, 1 cool, 2 normal}
```

sparse

- *NonSparseToSparse, SparseToNonSparse*
- *all classifiers accept sparse data as input*
- *… but some expand the data internally*
- *… while others use sparsity to speed up computation – e.g. NaiveBayesMultinomial, SMO*
- *StringToWordVector produces sparse output*

weighted instances

- *missing weights are assumed to be 1*

```
@data
sunny, 85, 85, FALSE, no, {0.5}
sunny, 80, 90, TRUE, no, {2.0}
…
```

date attributes

relational attributes (multi-instance learning)

Lesson 5.5: ARFF and XRFF

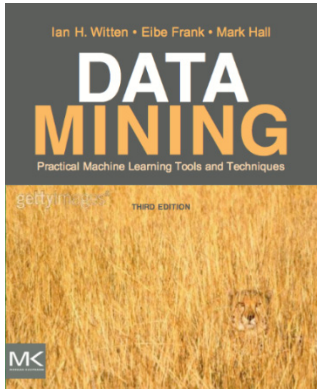
XML file format: XRFF

- Explorer can read and write XRFF files
- Verbose (compressed version: .xrff.gz)
- Same information as ARFF files
  - *including sparse option*
    and instance weights
- plus a little more
  - *can specify which attribute is the class*
  - *attribute weights*

```
<dataset name="weather.symbolic" version="3.6.10">
  <header>
    <attributes>
      <attribute name="outlook" type="nominal">
        <labels>
          <label>sunny</label>
          <label>overcast</label>
          <label>rainy</label>
        </labels>
      </attribute>
      …
  </header>
  <body>
    <instances>
      <instance>
        <value>sunny</value>
        <value>hot</value>
        <value>high</value>
        <value>FALSE</value>
        <value>no</value>
      </instance>
      …
    </instances>
  </body>
</dataset>
```

Lesson 5.5: ARFF and XRFF

- ARFF has extra features
  - sparse format
  - instance weights
  - date attributes
  - relational attributes
- Some filters and classifiers take advantage of sparsity
- XRFF is XML equivalent of ARFF
  - plus some additional features



Course text

- Section 2.4 *ARFF format*

More Data Mining with Weka

Class 5 – Lesson 6

Summary

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Lesson 5.6: Summary

Class 1 **Exploring Weka's interfaces; working with big data**

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Lesson 5.5 ARFF and XRFF

Lesson 5.6 Summary

Lesson 5.6 Summary

From *Data Mining with Weka*

- **There's no magic in data mining**
  - *Instead, a huge array of alternative techniques*
- **There's no single universal "best method"**
  - *It's an experimental science!*
  - *What works best on your problem?*
- **Weka makes it easy**
  - *... maybe too easy?*
- **There are many pitfalls**
  - *You need to understand what you're doing!*
- **Focus on evaluation ... and significance**
  - *Different algorithms differ in performance – but is it significant?*

Lesson 5.6 Summary

What did we miss in *Data Mining with Weka*?

- **Filtered classifiers**
  Filter training data but not test data – during cross-validation
- **Cost-sensitive evaluation and classification**
  Evaluate and minimize cost, not error rate
- **Attribute selection**
  Select a subset of attributes to use when learning
- **Clustering**
  Learn something even when there's no class value
- **Association rules**
  Find associations between attributes, when no "class" is specified
- **Text classification**
  Handling textual data as words, characters, n-grams
- **Weka Experimenter**
  Calculating means and standard deviations automatically … + more

Lesson 5.6 Summary

What did we do in *More Data Mining with Weka*?

- **Filtered classifiers** ✓
  Filter training data but not test data – during cross-validation
- **Cost-sensitive evaluation and classification** ✓
  Evaluate and minimize cost, not error rate
- **Attribute selection** ✓
  Select a subset of attributes to use when learning
- **Clustering** ✓
  Learn something even when there's no class value
- **Association rules** ✓
  Find associations between attributes, when no "class" is specified
- **Text classification** ✓
  Handling textual data as words, characters, n-grams
- **Weka Experimenter** ✓
  Calculating means and standard deviations automatically … + more

Plus …

- **Big data** ✓
- **CLI** ✓
- **Knowledge Flow** ✓
- **Streaming** ✓
- **Discretization** ✓
- **Rules vs trees** ✓
- **Multinomial NB** ✓
- **Neural nets** ✓
- **ROC curves** ✓
- **Learning curves** ✓
- **ARFF/XRFF** ✓

Lesson 5.6 Summary

What have we missed?

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  Environment for time series forecasting

- **Stream-oriented algorithms**

  MOA system for massive online analysis

- **Multi-instance learning**

  Bags of instances labeled positive or negative, not single instances

- **One-class classification**

- **Interfaces to other data mining packages**

  Accessing from Weka the excellent resources provided by the R data mining system

  Wrapper classes for popular packages like LibSVM, LibLinear

- **Distributed Weka with Hadoop**

- **Latent Semantic Analysis**

These are available as Weka “packages”

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Advanced Data Mining with Weka??

Lesson 5.6 Summary

- **“Data is the new oil”**
  - *economic and social importance of data mining will rival that of the oil economy (by 2020?)*
- **Personal data is becoming a new economic asset class**
  - *we need trust between individuals, government, private sector*
- **Ethics**
  - *“a person without ethics is a wild beast loosed upon this world”*
    … Albert Camus
- **Wisdom**
  - *the value attached to knowledge*
  - *“knowledge speaks, but wisdom listens” … attributed to Jimi Hendrix*

More Data Mining with Weka

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