# IRDS: Evaluation, Debugging, and Diagnostics

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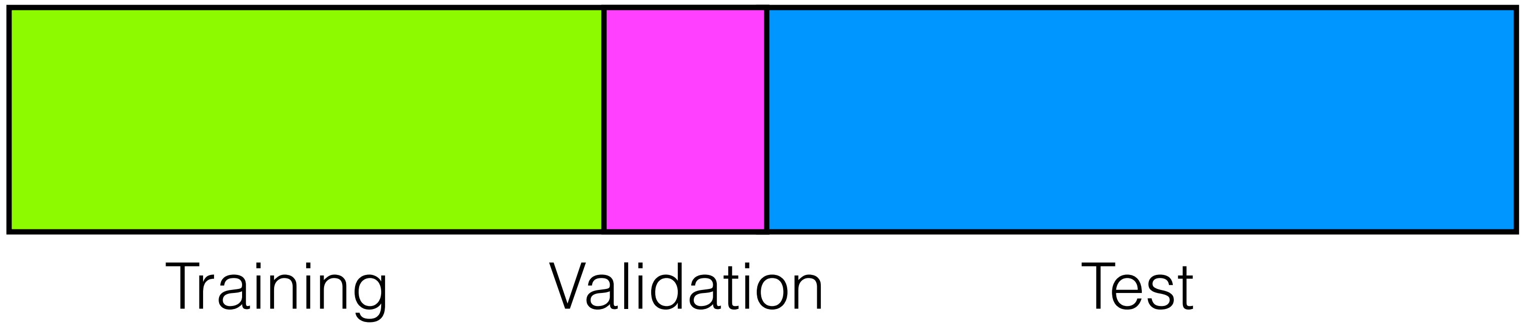
## Partitioning Data



Training : Running learning algorithms

Validation : Tuning parameters of learning algorithm

(e.g., regularization parameters)

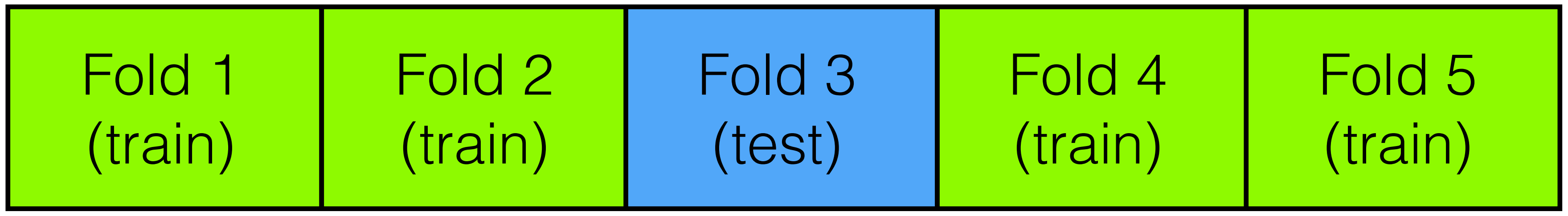
Test : Estimate performance on new situation

*ideally only used once…*

but this is never really possible

(research field overfitting!)

# Cross-Validation



Split data into *K* equal partitions

For each partition

    Train on all other

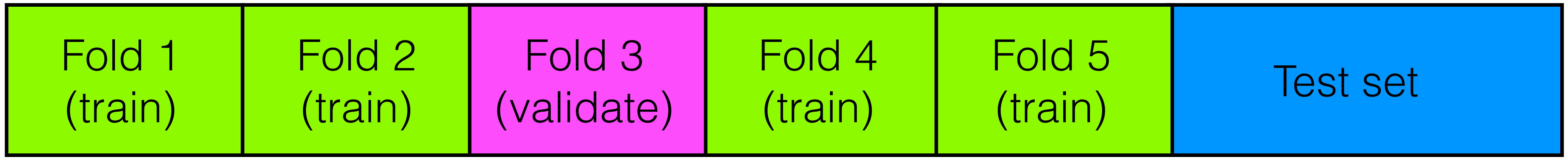
Average performance over *K* folds

This way every example is used an a test example

    (useful if data scarce)

# Cross-Validation

for parameter tuning (e.g., *k* in *k*-nearest neighbour)



```
First partition into training and test set
Then on training set only:
    For each value of parameter,
        e.g., k in {1,2,5,10,…}
        Run K-CV to estimate performance
    Train one model with best k on entire train set
```

# Measures for Regression

Root Mean Squared Error (RMSE)

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - f(x_i)\right)^2}$$

Test set denoted

$$\{(x_i, y_i) \mid i \in \{1, 2, \ldots N\}\}$$

Mean Absolute Error

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|y_i - f(x_i)\right|$$

Learned Regression function

$$f(x_i)$$

# Measures for Classification

## Accuracy

%age correctly labeled

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

## Precision

"when I say +, how often am I right?"

$$P = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

## Recall

of the real +, how many do I find?

$$R = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

| | | True label + | True label - |
|---|---|---|---|
| Predicted label | + | TP | FP |
| | - | FN | TN |

TP: True positives

Number of test instances where

true label == +, predicted label == +

FP: False positives

TN: True negatives

FN: False negatives

TP + FP + TN + FN = N

Total number of test instances

(for a multi-class problem, can compute P and R for each class)

## Interesting Facts about P, R

- Accuracy is a simple measure and a single number. This is good.
- Precision and recall can be interesting when
  - The classes are highly skewed
  - You want to understand performance on individual classes
    - One class more important, e.g., information retrieval
    - Many classes and want to break
  - You want to understand performance as a function of how “conservative” the predictions are.
- P and R are an interesting pair because they are in conflict
  - A good principle for pairs of evaluation measures

## Debugging and Diagnostics

Based on  slides from Stephen Gould and Andrew Ng

# What do I do now?

- You build a classifier (e.g., a spam filter using logistic regression) and the error is too high.
- What do you do to fix it? There are lots of things you could try:
  - Collect more training data.
  - Add different features (e.g., from the email header)
  - Try fewer features (e.g., exclude rare words from the classifier)
  - Try an SVM instead of logistic regression
  - Fix a bug in your stochastic gradient descent procedure
- You could do trial and error, but better is to think of **diagnostics**

# Bias-Variance Tradeoff

Let $\theta \in \mathbb{R}$ be some quantity we estimate by a random variable $\hat{\theta}$

Example:

$$\theta = \int xp(x)dx \qquad \hat{\theta} = \frac{1}{N}\sum_{i=1}^{N} x_i \qquad x_1 \ldots x_N \sim p$$

Define the *bias* and *variance*

$$\mathrm{Bias}(\hat{\theta}) = E(\theta - \hat{\theta}) = \theta - \mu$$

$$\mathrm{Var}(\hat{\theta}) = E\left[\hat{\theta} - \mu\right]^2$$

where $\mu = \iiint \hat{\theta}\, p(x_1, \ldots, x_N)\, dx_1 \cdots dx_N$

Both are averages across all data sets that we might have seen.

FUN to look up: Bias-variance decomposition

Useful concepts more generally. These trade off…

# Bias-Variance Tradeoff

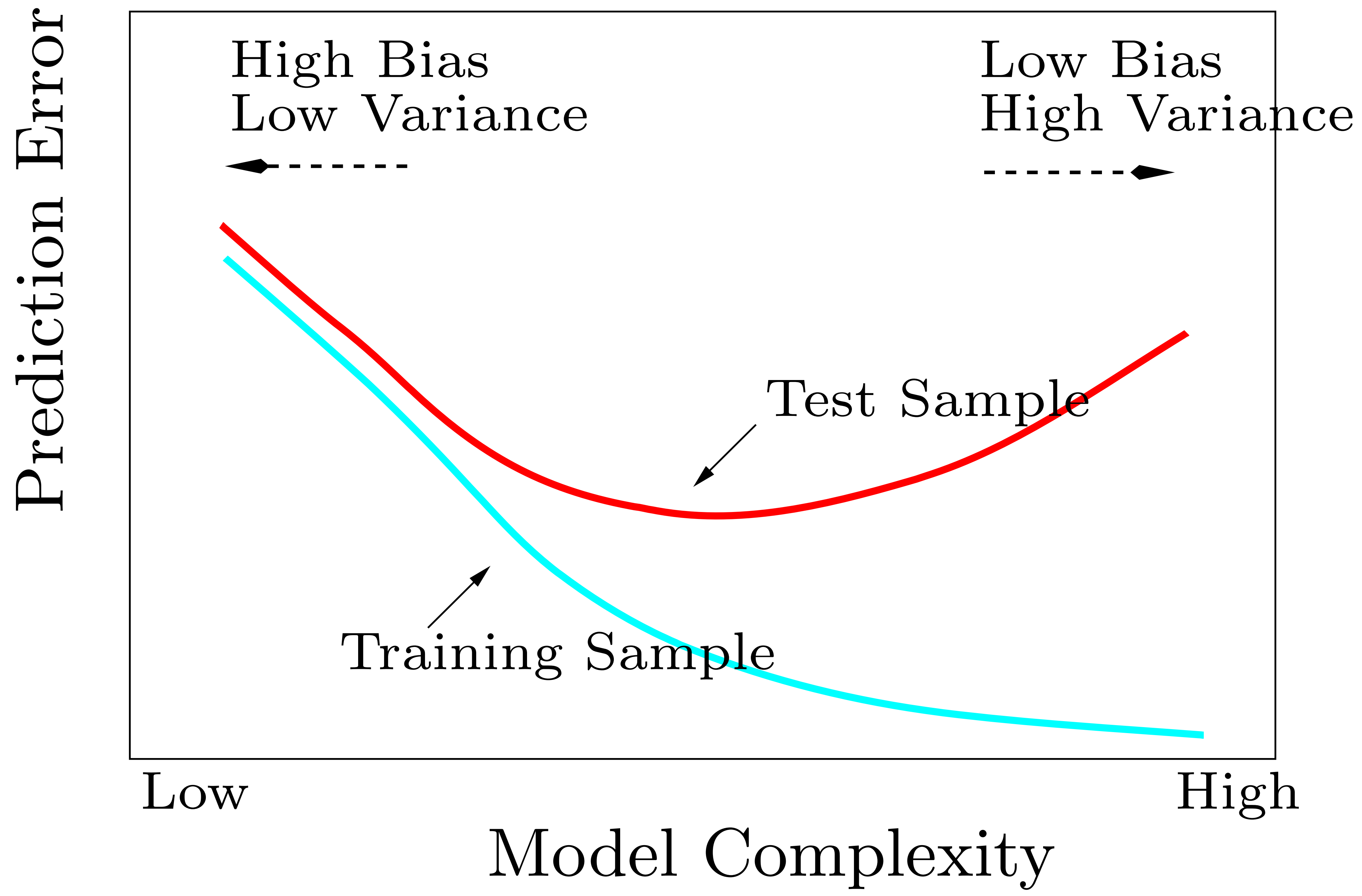
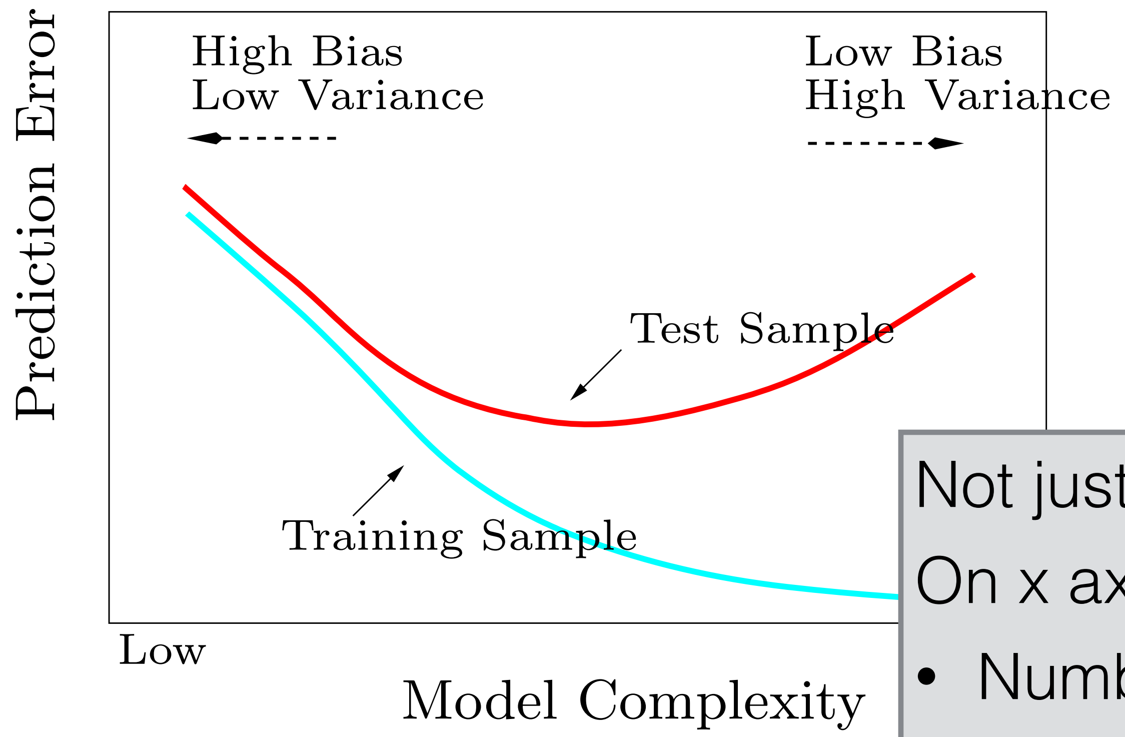


Figure from [Hastie, Tibshirani, and Friedman, 2009]

# Bias-Variance Tradeoff

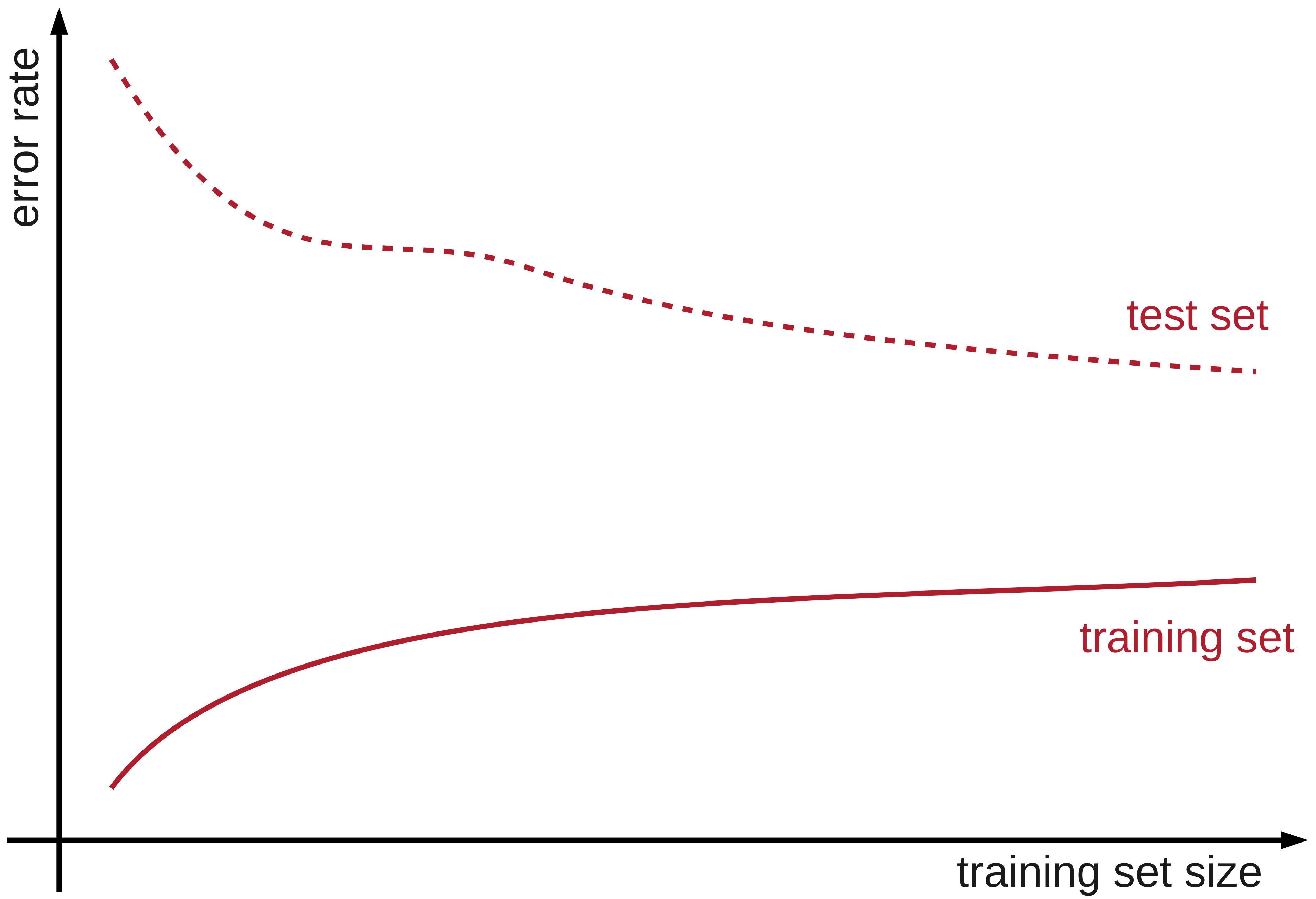


Not just a cartoon. Can use as a diagnostic.

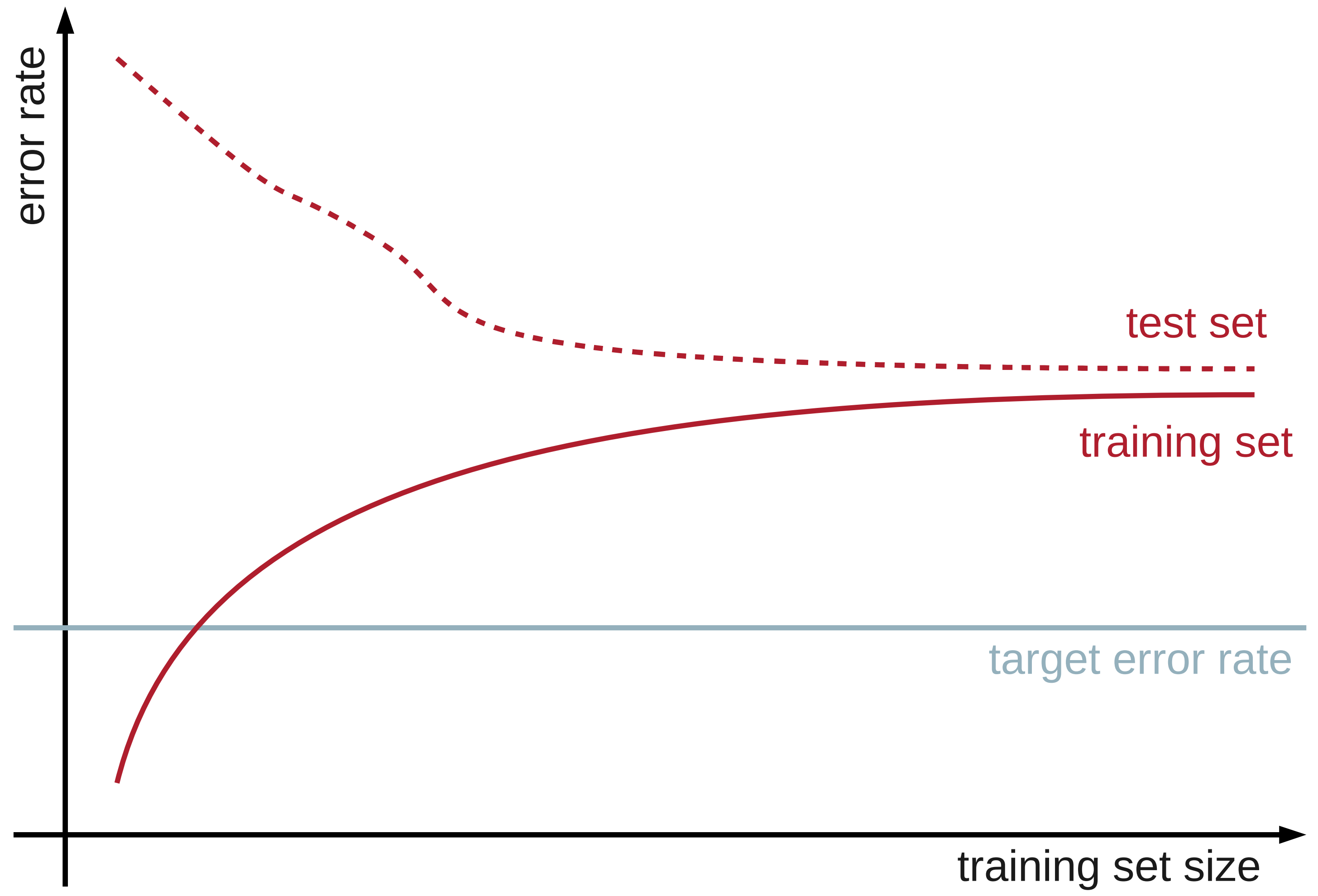
On x axis could put

- Number of features
  - (sort in some meaningful way)
- Model parameter that controls complexity
  - k in k-nearest neighbour
  - number of trees in boosting, random forests
  - regularization parameters
- Or perhaps you have access to more complex models
  - e.g., naive Bayes versus HMM

# Learning Curves



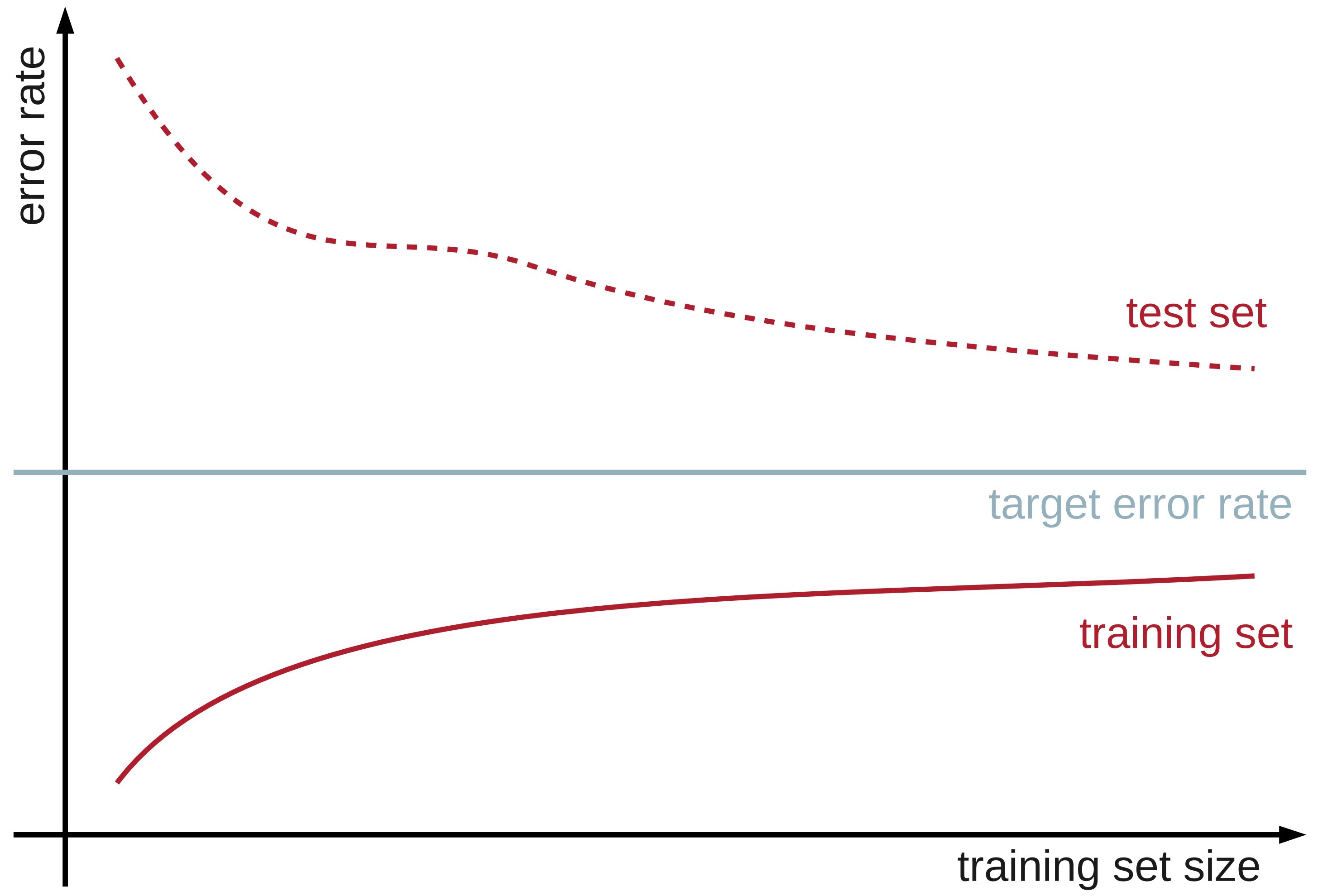
# Learning Curve Example 1



(Q: Why is error going up?)
Test error no longer decreasing
Even training error is too high
Not much difference between training and test error

high bias

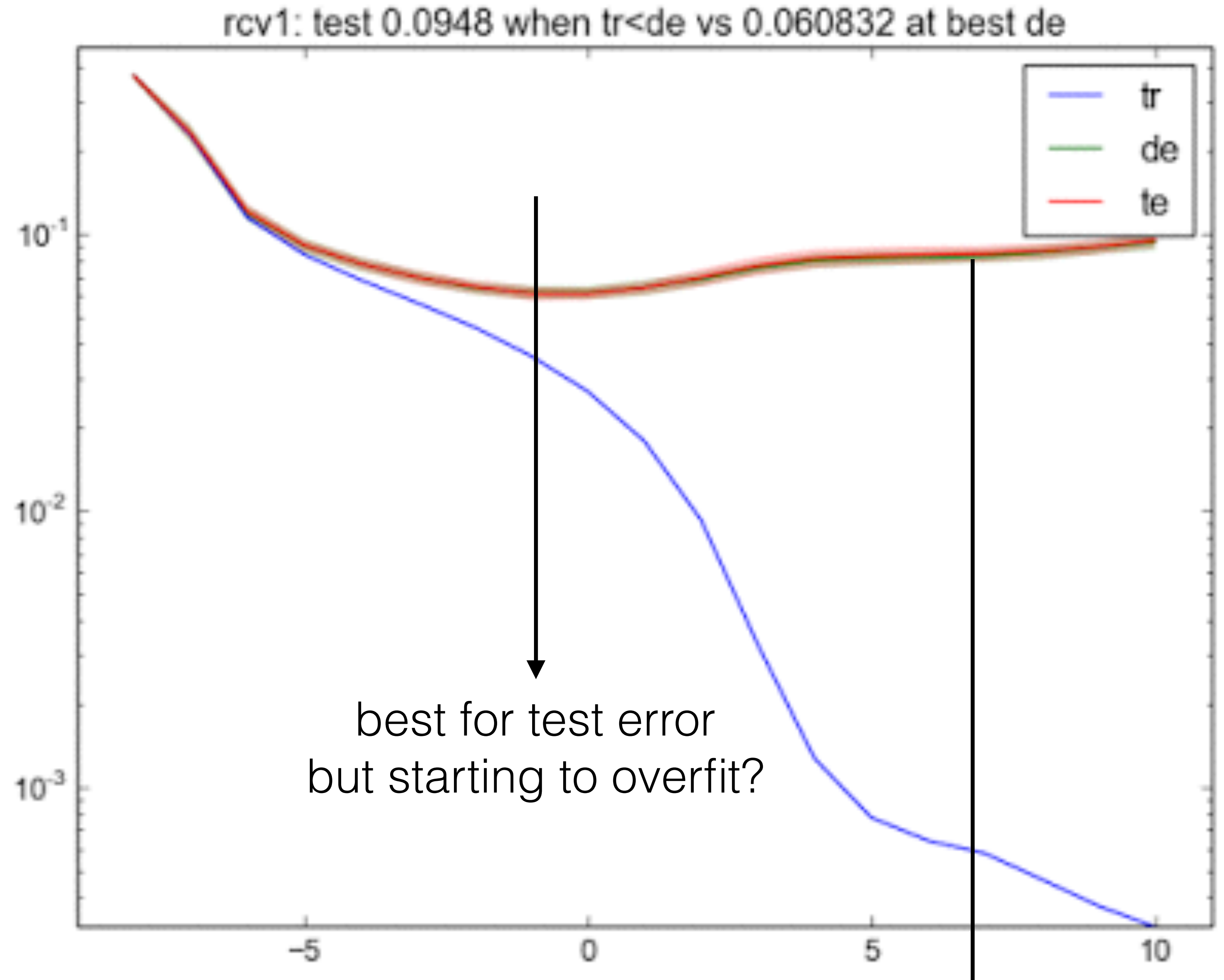
# Learning Curve Example 2



high variance

Test error still decreasing
Big gap training and test error

## Zero Overfitting Not Desirable



error

best for test error
but starting to overfit?

regularization

definitely overfitting

http://nlpers.blogspot.co.uk/2015/09/overfitting.html

# Optimization in the Loop

- Often learning methods work by optimizing some objective function.
- For example, recall logistic regression

$$p(y = 1|\mathbf{x}) = \frac{1}{1 + \exp\{-\mathbf{w}^\top \mathbf{x}\}}$$

- To learn the weights, we solve

$$\max_{\mathbf{w}} L(\mathbf{w}) = \sum_{i=1}^{N} \log p(y = y^{(i)}|\mathbf{x} = \mathbf{x}^{(i)})$$

$$\text{data points } (\mathbf{x}^{(i)}, y^{(i)}) \text{ for } i \text{ in } 1 \ldots N$$

- Maybe optimise this using gradient descent
- When this performs poorly, now have two questions
  - Is my numerical optimization algorithm performing poorly?
  - Or is objective function *L* not doing what I want?
    - (Simple ex: spam filtering with cost-sensitive error)
- Comes up especially often during **research** in data science
  - Often we introduce new models (== new objective function)
  - Which might be harder to optimize

# Optimization Example

Example: To optimize

$$\max_{\mathbf{w}} L(\mathbf{w}) = \sum_{i=1}^{N} \log p(y = y^{(i)} | \mathbf{x} = \mathbf{x}^{(i)})$$

Simple choice is batch gradient descent:

$$\nabla_{\mathbf{w}} L(\mathbf{w}) = \sum_{i=1}^{N} \nabla_{\mathbf{w}} \left[\log p(y = y^{(i)} | \mathbf{x} = \mathbf{x}^{(i)})\right]$$

This will be slow if *N* is big.

Alternative: *stochastic gradient descent*.
Simplest version: Sample $i \sim \mathrm{Uniform}(\{1, 2, \ldots, N\})$

Compute $\nabla_{\mathbf{w}} \log p(y = y^{(i)} | \mathbf{x} = \mathbf{x}^{(i)})$ (single instance!)

Update using this gradient.
(this is standard in deep learning, e.g.)

# Optimization Diagnostic

- You run a logistic regression spam filter on 100,000 training instances. $\mathbf{w}^*_{\mathrm{GD}}$
  - Using batch gradient descent, you get an accuracy of 85%
- Not good enough, so you get a larger set of 100,000,000 examples $\mathbf{w}^*_{\mathrm{SGD}}$
  - Batch gradient is too slow, so you switch to SGD
  - Now you only get 80% accuracy (!?!?)

## Diagnostic: Check the batch **training** objective

$$L(\mathbf{w}) = \sum_{i=1}^{100\,000\,000} \log p(y = y^{(i)} | \mathbf{x} = \mathbf{x}^{(i)})$$

Compute this for final result of batch GD $\mathbf{w}^*_{\mathrm{GD}}$ and SGD $\mathbf{w}^*_{\mathrm{SGD}}$

If $L(\mathbf{w}^*_{\mathrm{SGD}}) \leq L(\mathbf{w}^*_{\mathrm{GD}})$

then your SGD procedure is screwed up
(maybe try a different step size?)

This kind of thing happens far more generally.

# The Numerical Gradient Check

- Often optimization packages require you to implement functions for both

$$\mathbf{w} \mapsto L(\mathbf{w}) \qquad\qquad \mathbf{w} \mapsto \nabla_{\mathbf{w}} L$$

  - (although automatic differentiation is becoming more popular)
- In that case, check whether

$$\epsilon^{-1} L(\mathbf{w} + \epsilon) - L(\mathbf{w}) = \nabla_{\mathbf{w}} L$$

- Easy to have a bug in one function but not the other.
- Do this for different settings of $\mathbf{w}$
- MATLAB does this automatically if you ask it to…

# Nested Models

- Often complicated models *contain* simpler models as a special case. For logistic regression:

$$p(y = 1|\mathbf{x}) = \frac{1}{1 + \exp\{-\mathbf{w}^\top \mathbf{x}\}}$$

- so if **w** = 0, the distribution over *y* is be uniform. Is that what happens in your code? If not, bug.
- Another example: a hidden Markov model and a mixture model

$$p(\mathbf{x}, \mathbf{z}) = \prod_t p(x_t|z_t)p(z_t|z_{t-1})$$

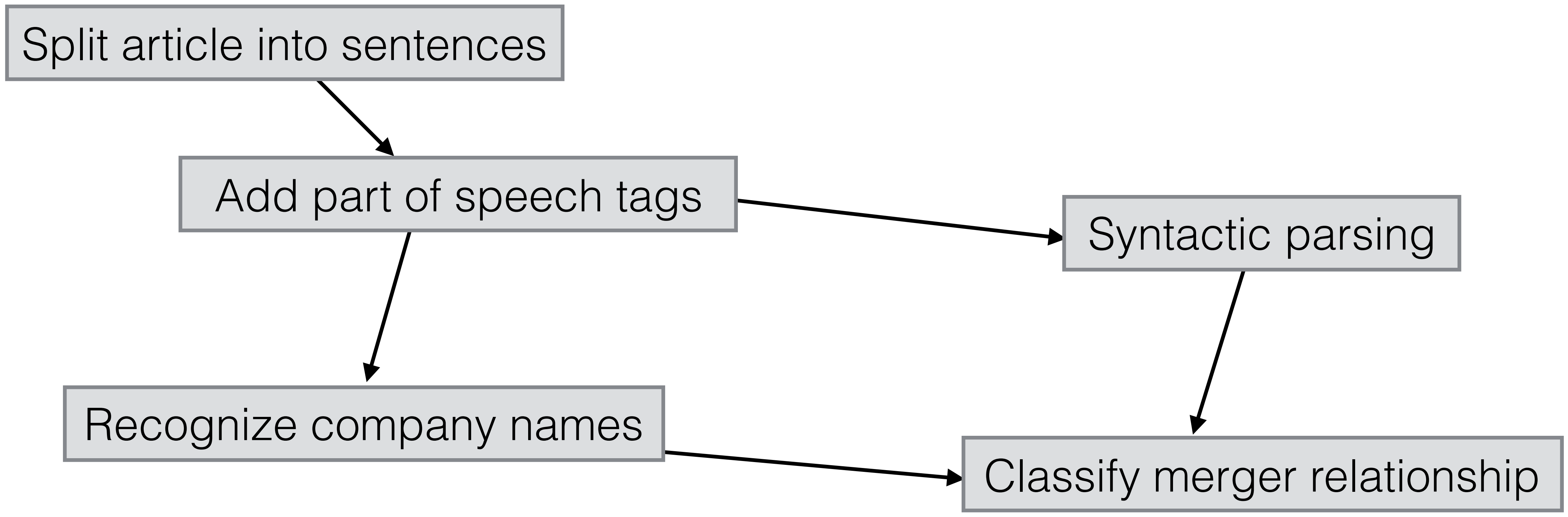
$$\text{if } p(z_t|z_{t-1}) \text{ ignores } z_{t-1}, \text{ then all } x_t \text{ independent ... mixture model}$$

- Lots of ways to get diagnostics from this:
  - Training error of HMM should be strictly better
  - Force your HMM code to fit observation distributions only.
    - Do you get the same distribution as mixture model
  - Logistic regression: Numerical gradient check
    - Try it first at **w**=0. It will be easier to debug there.

# Pipelines of Predictions

Practical systems use predictors at multiple points

e.g., Finding company mergers from newswire text



Many steps rely on learning, will make errors
Is one step a weak link? Or are errors slowly propagating?

Debug by replacing intermediate predictions
with gold standard (human annotations)

# Overall Advice

- For practical work: Try quick and dirty first. Iterate quickly
- Different diagnostics
    - Learning curves
        - As function of size of training set
        - As function of model complexity
        - Additionally: number of iterations of learning algorithm
    - Optimization diagnostics
    - Diagnostics using model nesting
    - Breaking chains of predictions
- Sometimes diagnostics require a bit of ingenuity.
- “Trust no one”
    - Just because something is true in the maths doesn’t mean it is in your code
    - Imagine how you think the method is probably behaving and check whether that happens!
    - (this holds for research too!)