THE UNIVERSITY *of* EDINBURGH
informatics

Applied Machine Learning (AML)

Model Selection

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Direct Comparison

Comparing Evaluation Measures

email
"send us your password"
"send us review"
"review your account"
"review us"
"send your password"
"send us your account"
⋮

Comparing Evaluation Measures

email	true
"send us your password"	+
"send us review"	−
"review your account"	−
"review us"	+
"send your password"	+
"send us your account"	+
⋮	

Acc
κ
F1-score
ROC AUC
⋮

Comparing Evaluation Measures

email	true	pred (A)
"send us your password"	+	+
"send us review"	−	+
"review your account"	−	−
"review us"	+	−
"send your password"	+	+
"send us your account"	+	+
⋮		

	Naive Bayes (A)
Acc	72.6%
κ	54.1%
F1-score	85.6%
ROC AUC	48.4%
⋮	⋮

Comparing Evaluation Measures

email	true	pred (A)	pred (B)
“send us your password”	+	+	+
“send us review”	–	+	–
“review your account”	–	–	+
“review us”	+	–	–
“send your password”	+	+	+
“send us your account”	+	+	–
⋮			

	Naive Bayes (A)	Logistic Regression (B)
Acc	72.6%	84.5%
κ	54.1%	66.2%
F1-score	85.6%	89.1%
ROC AUC	48.4%	55.7%
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Should we choose B over A?

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Should we choose B over A? maybe?

Comparing Point Estimates

$$\mathcal{D} = \{\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}}\} \qquad \mathcal{D}_{\text{train}} \cap \mathcal{D}_{\text{test}} = \emptyset$$

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Acc	79.3%	$>$	78.1%
κ	61.9%	$>$	60.3%
F1-score	86.1%	$>$	82.4%
ROC AUC	50.1%	$<$	50.4%
⋮	⋮		⋮

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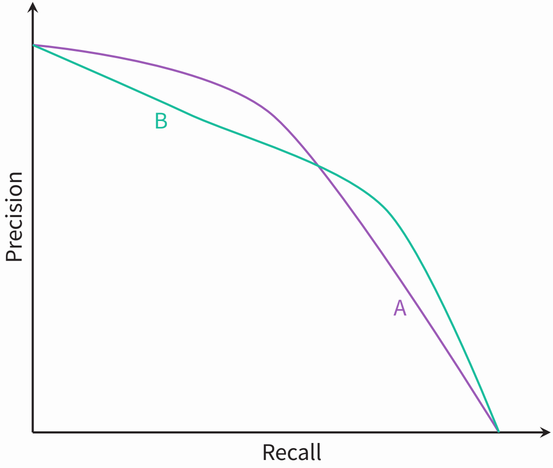
Point estimates can be susceptible to many kinds of random effects!

Comparison with Tradeoff



AUC of Precision-Recall

- Which model is better?

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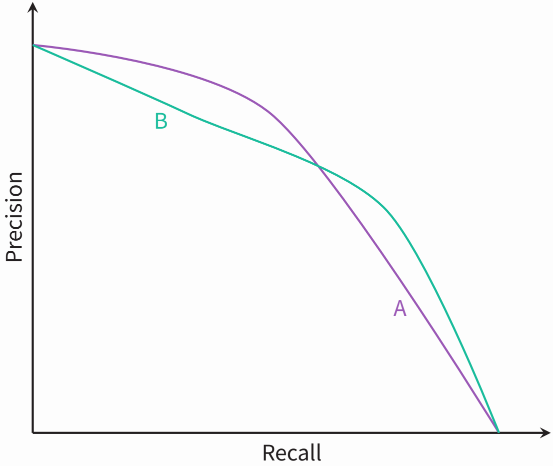

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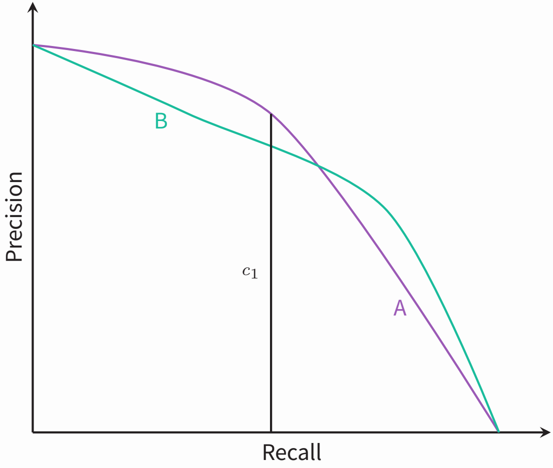

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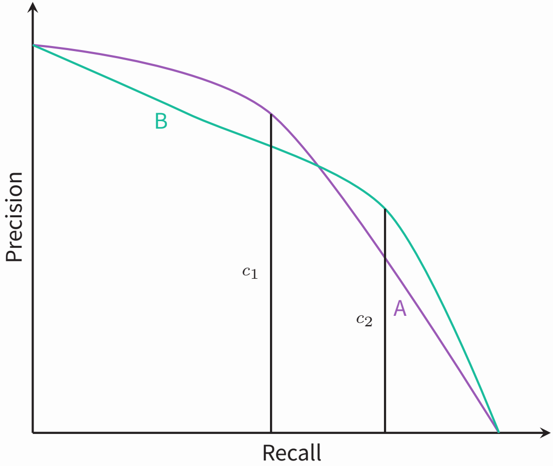

AUC of Precision-Recall

- Which model is better?
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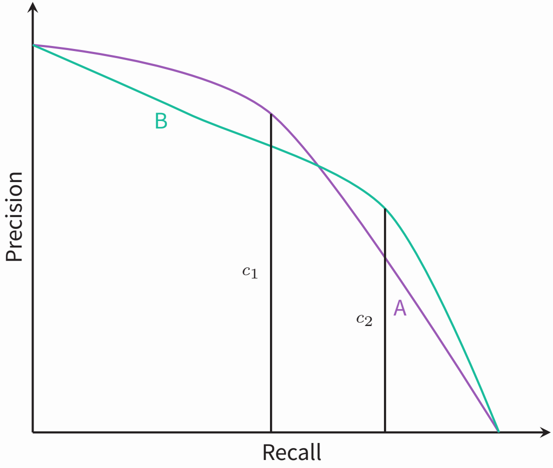

AUC of Precision-Recall

- Which model is better?
- Choice can depend on trade-off
  - lower recall, higher precision (c_1): $A > B$
  - lower precision, higher recall (c_2): $B > A$
- Random effects (e.g. data split) can make comparison hard

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Variation in error

- Dataset partitioning (e.g. cross validation)

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$$y_i = w_0 + w_1 x_i + \epsilon_i \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

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- Model (e.g. stochastic linear regression)

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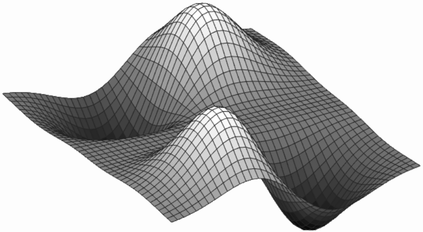
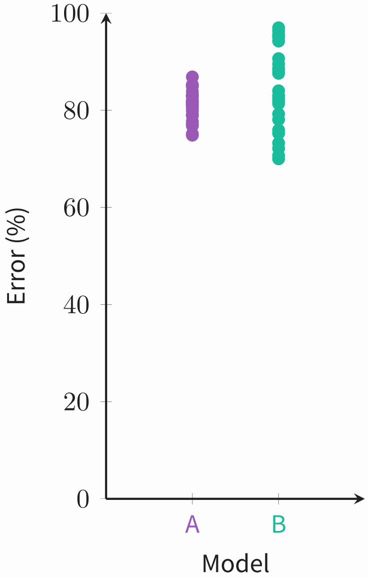
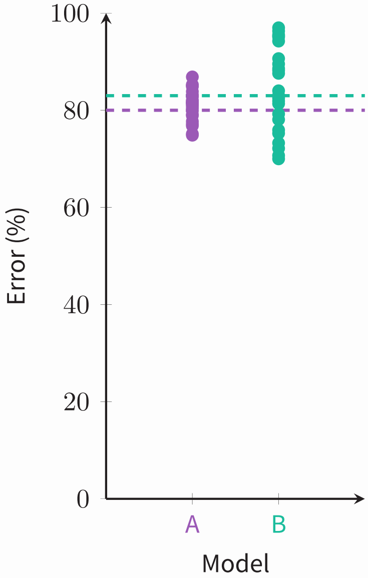
- Learning algorithm (e.g. SGD)
  - initialisation effects
  - local minima



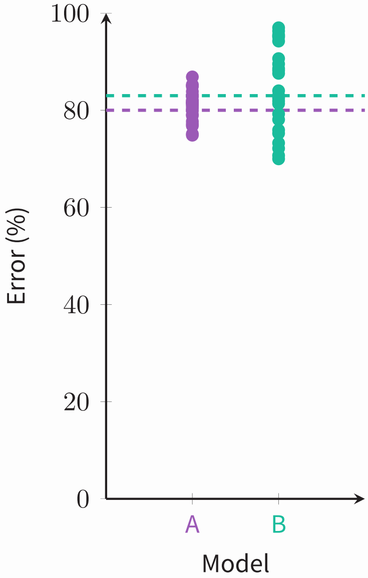
Comparing Distributions





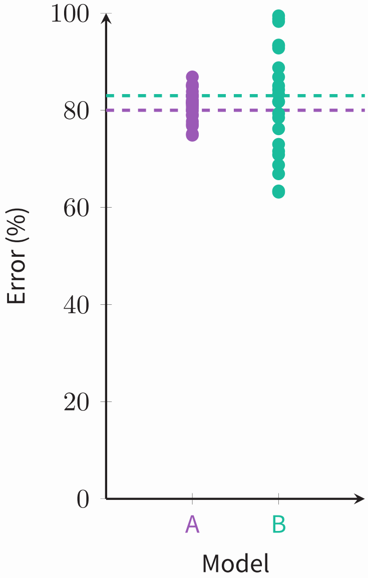
Comparing Distributions

- Compute the difference in *mean* error



Comparing Distributions

- Compute the difference in *mean* error
  - what difference is enough to decide B> A?



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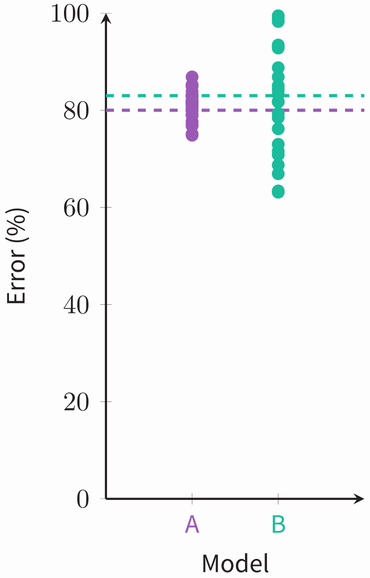

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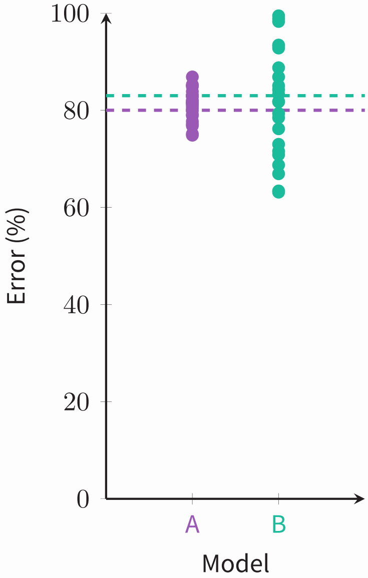

Comparing Distributions

- Compute the difference in *mean* error
  - what difference is enough to decide B> A?
  - does the spread / variance affect this choice?
- Difficult to provide a general approach to say one model is "better" than another
- Weaker, but feasible, approach:

  How likely is it that the observed disparities are due to chance?

Statistical Tests

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Population vs. Sample statistics

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Population: All the elements from a set

E.g. All leave-1-out splits of the dataset

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Population: All the elements from a set

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Sample: Observations drawn from population

E.g. Some N splits of the dataset

If sample set is $x_1, \ldots, x_N$

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2$$

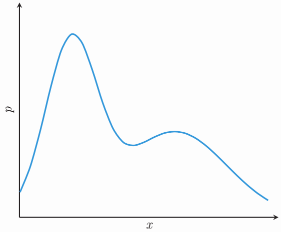
*Bessel's correction

Preliminaries

Central Limit Theorem (CLT)

For a set of samples $x_1, \ldots, x_N, \ldots$ from a population with expected mean μ and finite variance σ^2

$$z = \frac{\bar{x} - \mu}{\sigma / \sqrt{N}} \sim \mathcal{N}(0, 1) \quad \text{as } N \to \infty$$



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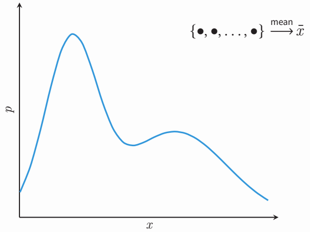

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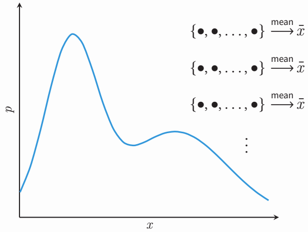

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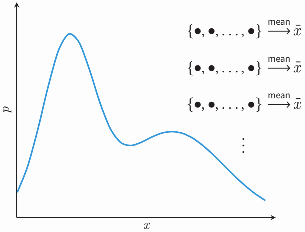

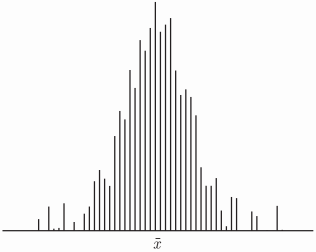

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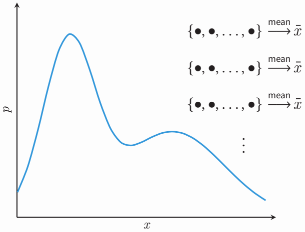

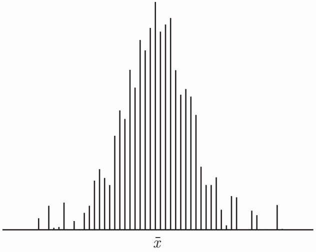

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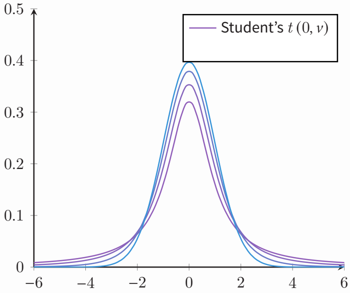

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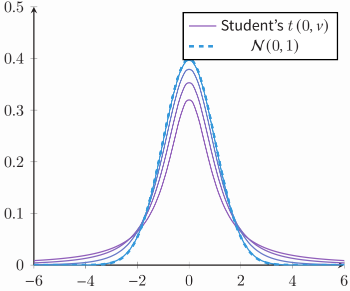

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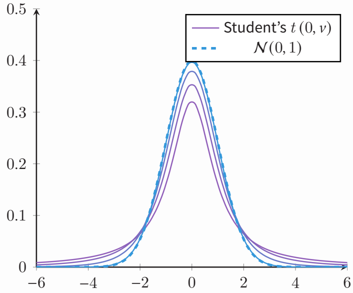

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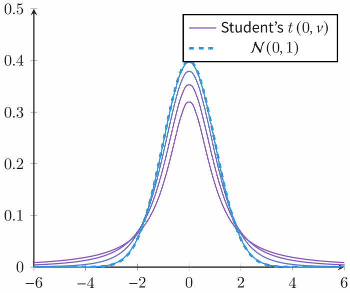

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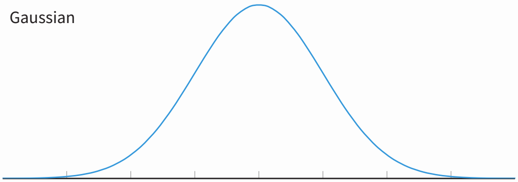

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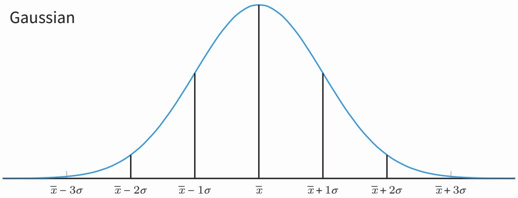

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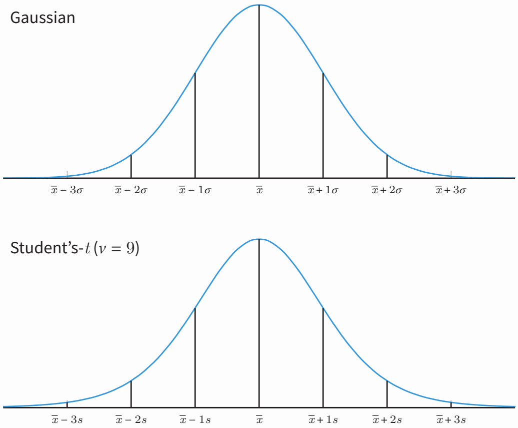

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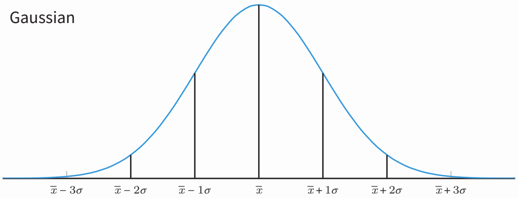
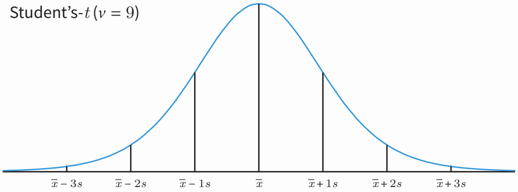
A common framework to evaluate chance occurrence.





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Hypothesis Testing

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- Mutually exclusive and exhaustive: $H_0 = \texttt{True} \implies H_1 = \texttt{False}$

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True \ Decision (Retain)	H_0	H_1
H_0	✓	Type II
H_1	Type I	✓

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Example: Hypothesis Testing for Models

Generating Variation

Data Split	A	B
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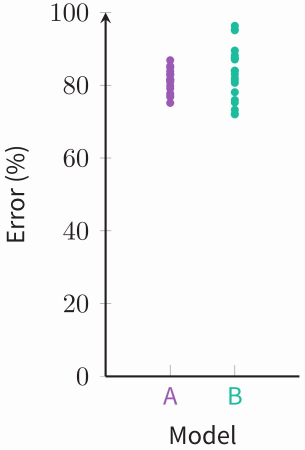
$\vdots$	$\vdots$	$\vdots$
$\{\mathcal{D}^N_{\text{train}}, \mathcal{D}^N_{\text{test}}\}$	ℓ^A_N	ℓ^B_N



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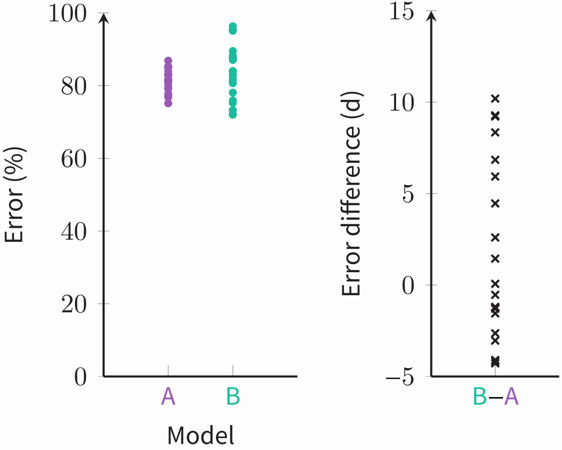

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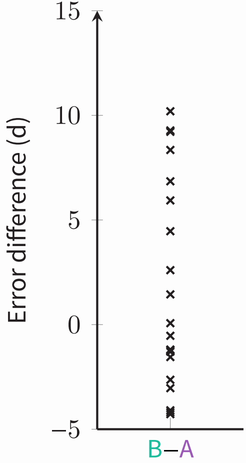

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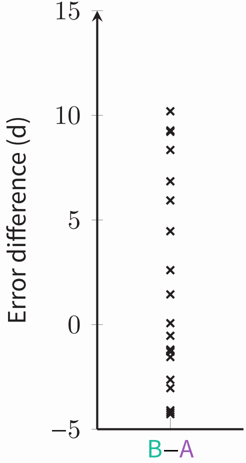

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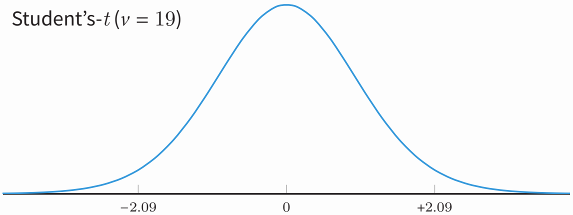

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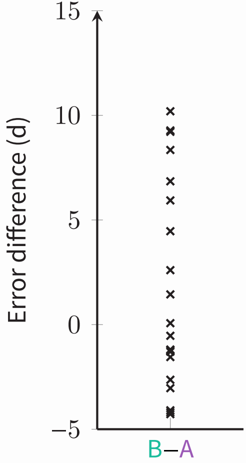

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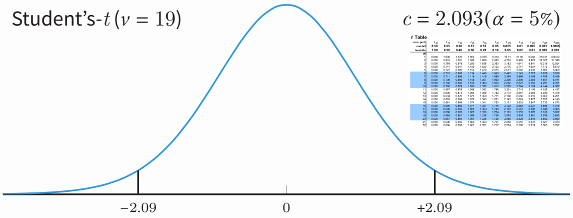

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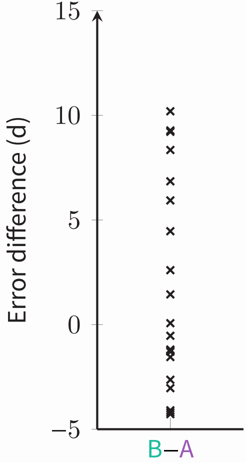

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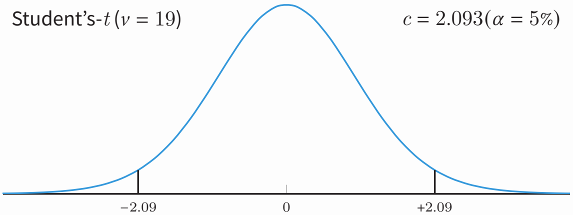
Student's-t $(\nu = 19)$ $\qquad c = 2.093 (\alpha = 5\%)$



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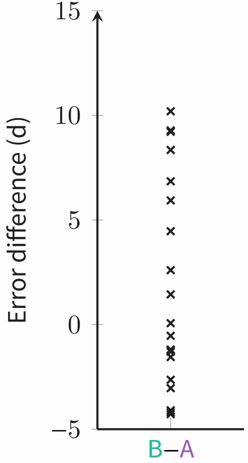

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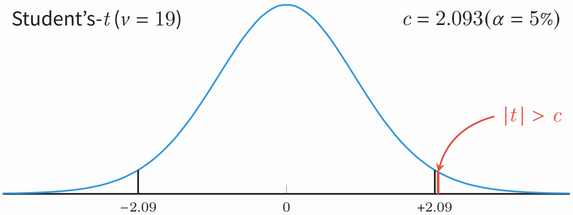

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  - **Remedy:** Report confidence interval (CI)

$$\bar{d} \pm c|_{\alpha/2} \cdot \frac{s}{\sqrt{N}}$$

which, for our example would be

$$2.53 \pm 2.093 \cdot \frac{5.27}{\sqrt{20}} \qquad (\alpha = 0.05,\ c|_{0.05} = 2.093)$$

$$2.53 \pm 2.47$$

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- **Solutions:**
  - 5x2 Cross Validation [1]
  - Adjust standard deviation to account for imbalance [2]
  - …and many more (ANOVA, Non-parametric tests, etc.)!

1. T. G. Dietterich, Approximate Statistical Tests for Comparing Supervised Classification Learning Algorithms, 1998
2. C. Nadeau & Y. Bengio, Inference for the Generalization Error, 2003

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Being able to compare models and experiments is both a science and an art!

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Being able to compare models and experiments is both a science and an art!

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- Some measures incorporate context; use it! (P-R, ROC)
- For when statistical tests are required (not always!)
  - ensure your assumptions on the model / data are clearly stated
  - ensure assumptions of the test are met
- Performance on error measures not all—speed, use of resources, and ease of implementation can, and should, affect preference!