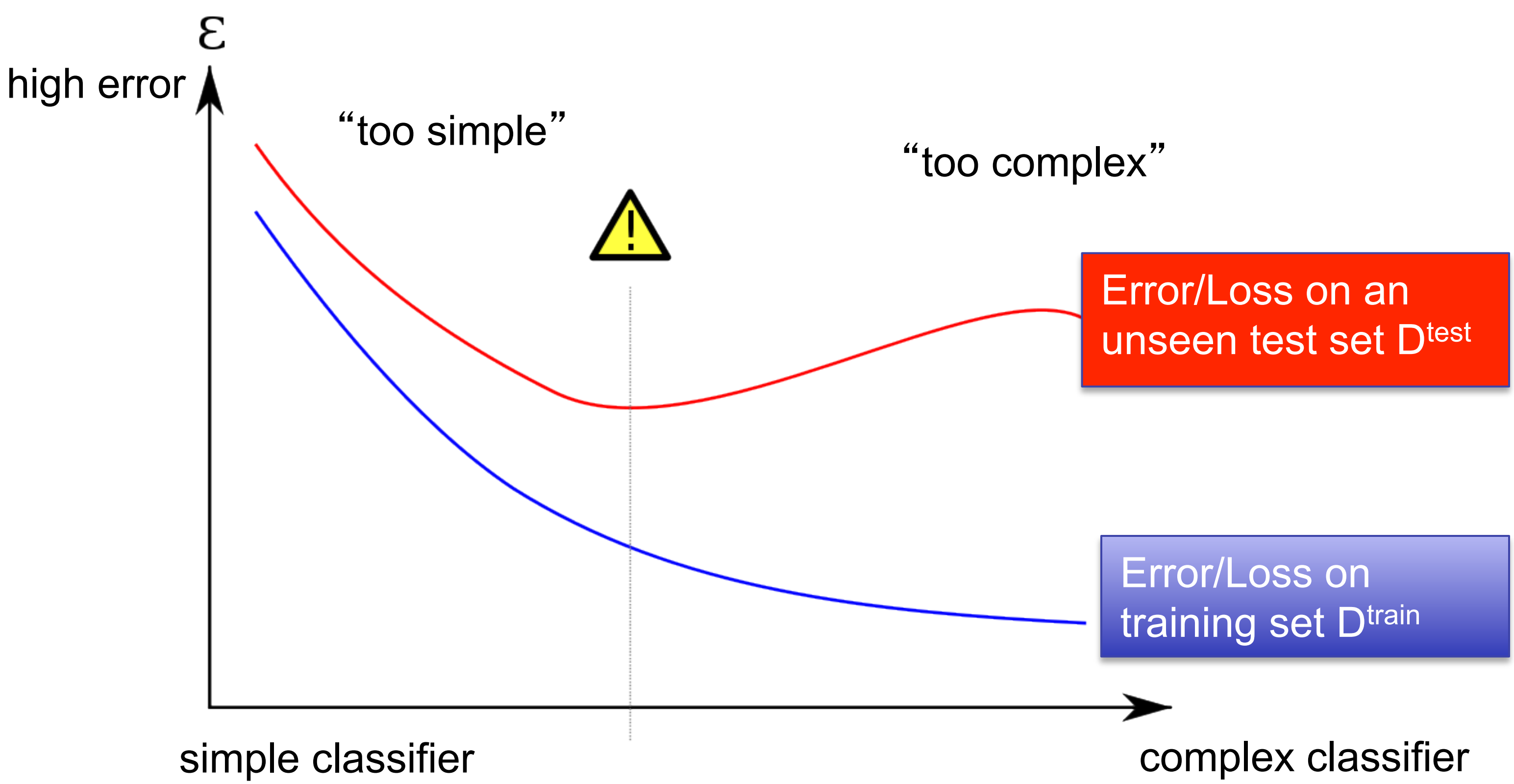
Bias-Variance in Machine Learning

Bias-Variance: Outline

- Underfitting/overfitting:
  - Why are complex hypotheses bad?
- Simple example of bias/variance
- Error as bias+variance for regression
  - brief comments on how it extends to classification
- Measuring bias, variance and error
- Bagging - a way to reduce variance
- Bias-variance for classification

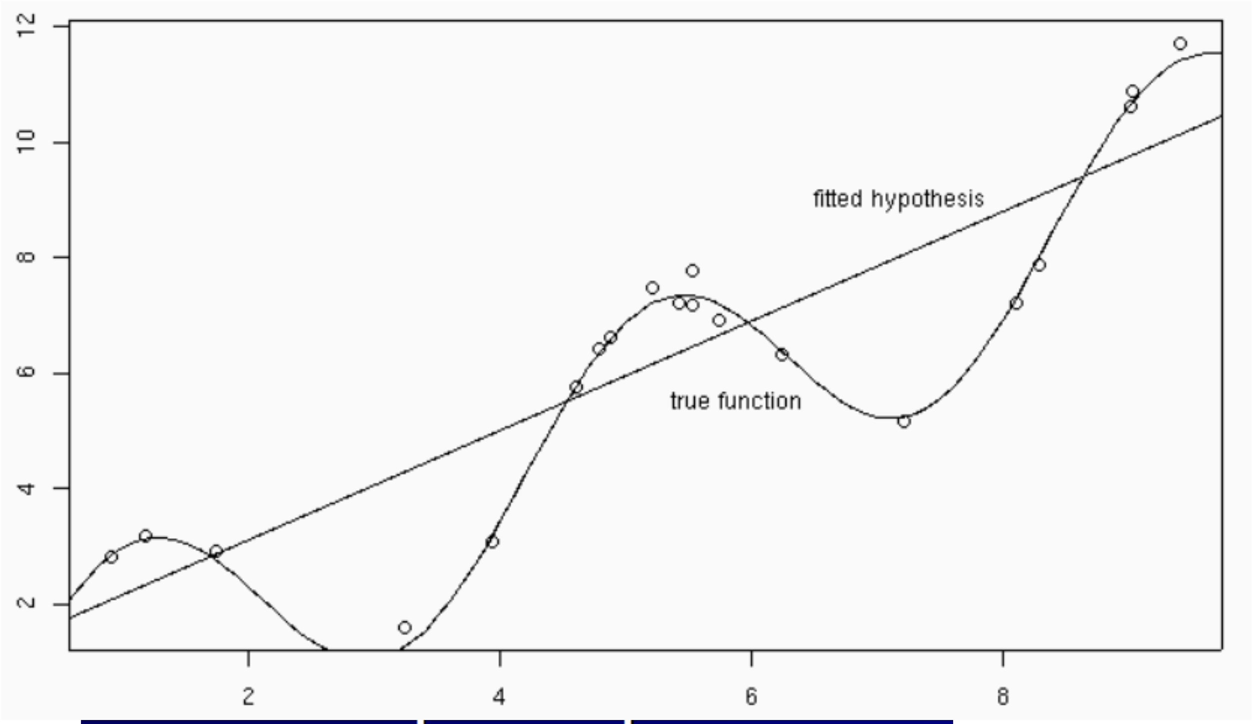
Bias/Variance is a Way to Understand Overfitting and Underfitting



Bias-Variance: An Example

Example

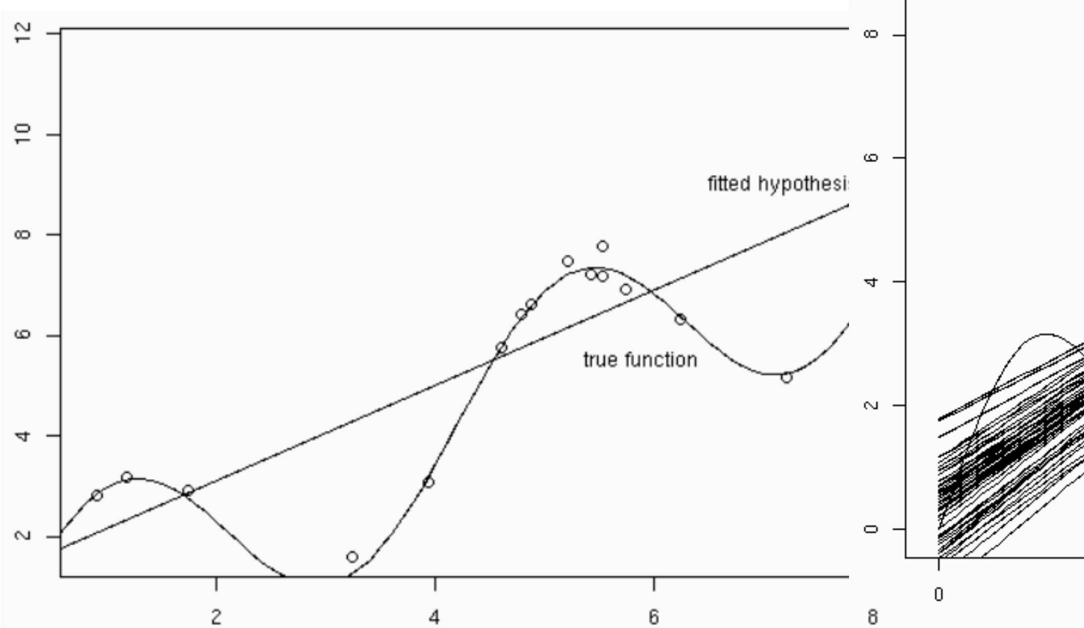
Tom Dietterich, Oregon St



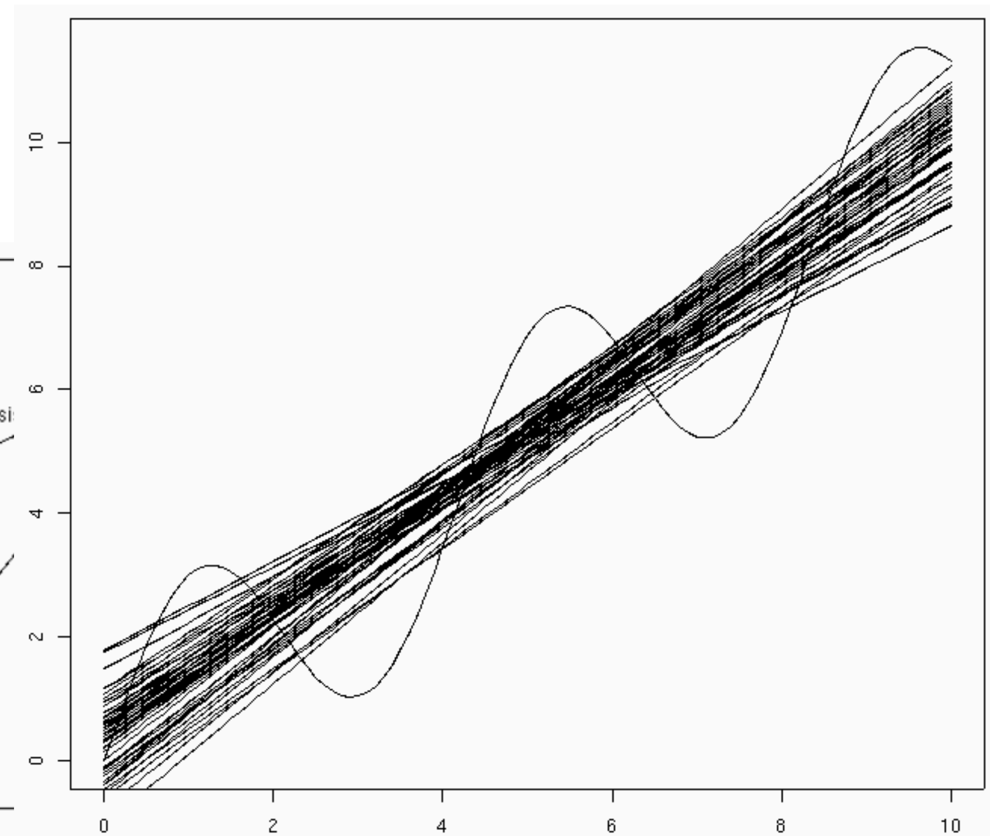
$y = x + 2\sin(1.5x) + N(0,0.2)$

Example

Tom Dietterich, Oregon St

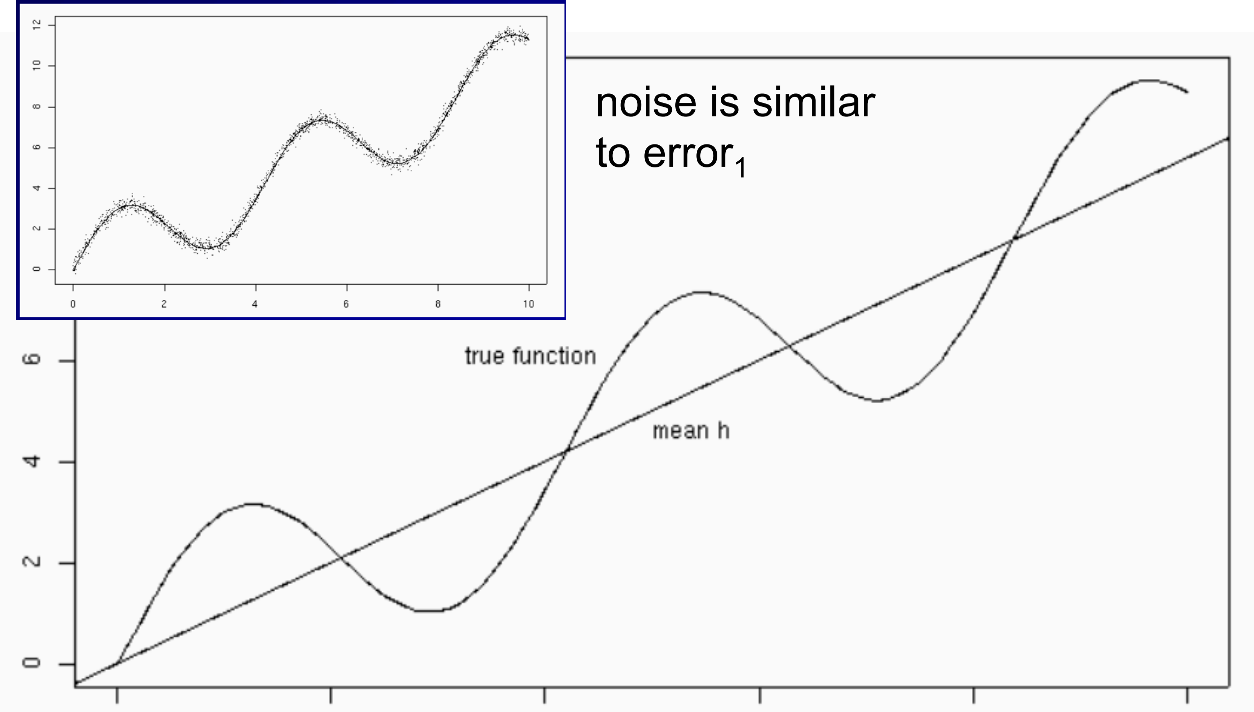


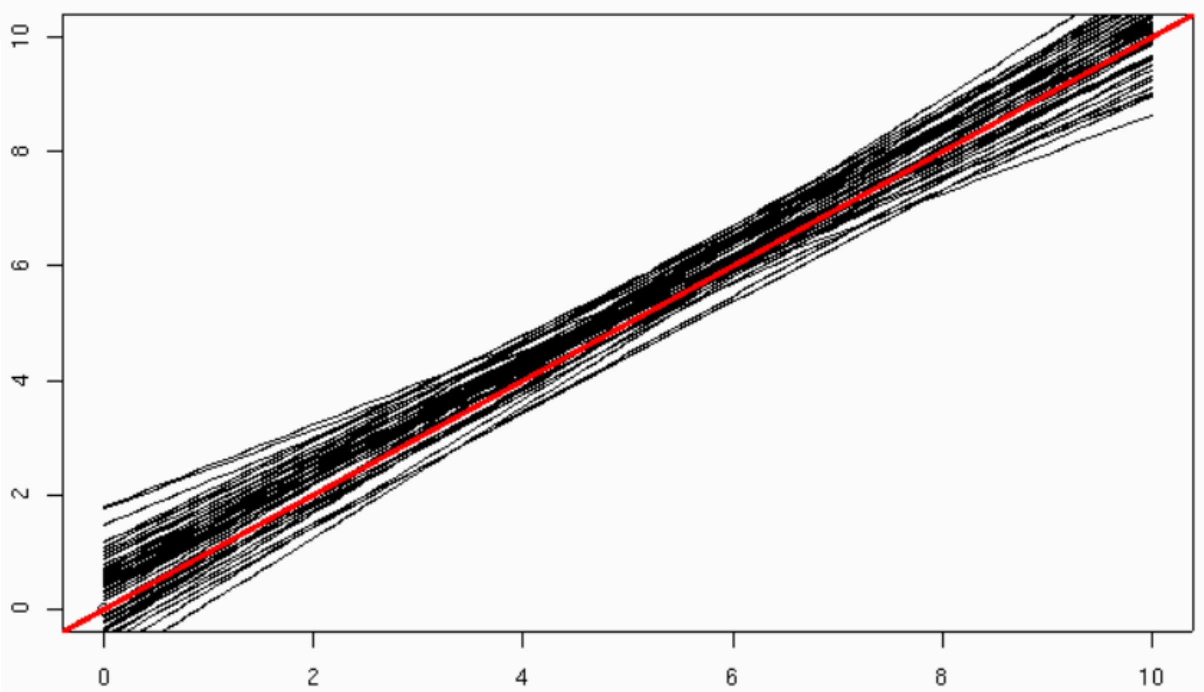
y = x + 2 sin(1.5x) + N(0,0.2)



Same experiment, repeated:
with 50 samples of 20 points each

noise is similar to $error_1$





The true function *f* can't be fit perfectly with hypotheses from our class *H* (lines) ➔ Error_1

Fix: *more* expressive set of hypotheses *H*

We don't get the best hypothesis from *H* because of noise/small sample size ➔ Error_2

Fix: *less* expressive set of hypotheses *H*

Bias-Variance Decomposition: Regression

Bias and variance for regression

- For regression, we can easily **decompose** the error of the learned model into two parts: bias (error 1) and variance (error 2)
  - Bias: the class of models **can't** fit the data.
    - **Fix**: a *more expressive* model class.
  - Variance: the class of models **could** fit the data, but doesn't because it's hard to fit.
    - **Fix**: a *less expressive* model class.

Bias – Variance decomposition of error

$$E_{D,\varepsilon}\left\{\left(f(x)+\varepsilon-h_D(x)\right)^2\right\}$$

dataset and noise

true function

noise

learned from D

Fix test case *x*, then do this experiment:

1. Draw size *n* sample D=$(x_1,y_1),\ldots.(x_n,y_n)$
2. Train linear regressor h_D *using* D
3. Draw one test example $(x, f(x)+\varepsilon)$
4. Measure squared error of h_D on that example *x*

What's the expected error?

Bias – Variance decomposition of error

Notation - to simplify this

$$f \equiv f(x) + \varepsilon \qquad \hat{y} = \hat{y}_D \equiv h_D(x)$$

$$E_{D,\varepsilon}\left\{ \left(f(x) + \varepsilon - h_D(x)\right)^2 \right\}$$

dataset and noise

true function

noise

learned from D

$$h \equiv E_D\{h_D(x)\}$$

long-term expectation of learner's prediction on this *x* averaged over many data sets *D*

Bias – Variance decomposition of error

$$h \equiv E_D\{h_D(x)\}$$
$$\hat{y} = \hat{y}_D \equiv h_D(x)$$
$$f \equiv f(x) + \varepsilon$$

$$E_{D,\varepsilon}\left\{ (f-\hat{y})^2 \right\}$$
$$= E\left\{ \left([f-h]+[h-\hat{y}]\right)^2 \right\}$$
$$= E\left\{ [f-h]^2 + [h-\hat{y}]^2 + 2[f-h][h-\hat{y}] \right\}$$
$$= E\left\{ [f-h]^2 + [h-\hat{y}]^2 + 2[fh - f\hat{y} - h^2 + h\hat{y}] \right\}$$
$$= E[(f-h)^2] + E[(h-\hat{y})^2] + 2\left(\cancel{E[fh]} - \cancel{E[f\hat{y}]} - \cancel{E[h^2]} + \cancel{E[h\hat{y}]}\right)$$

$$E_{D,\varepsilon}\left\{\left(f(x)+\varepsilon\right) * E_D\left\{h_D(x)\right\}\right\}$$
$$= E_{D,\varepsilon}\left\{\left(f(x)+\varepsilon\right) * h_D(x)\right\}$$

$$E_{D,\varepsilon}\left\{E_D\left\{h_D(x)\right\} * E_D\left\{h_D(x)\right\}\right\}$$
$$= E_{D,\varepsilon}\left\{E_D\left\{h_D(x)\right\} * h_D(x)\right\}$$

Bias – Variance decomposition of error

$$E_{D,\varepsilon}\left\{ (f-\hat{y})^2 \right\}$$
$$= E\left\{ \left([f-h]+[h-\hat{y}]\right)^2 \right\}$$
$$= E\left\{ [f-h]^2+[h-\hat{y}]^2+2[f-h][h-\hat{y}] \right\}$$
$$= E[(f-h)^2]+E[(h-\hat{y})^2]$$

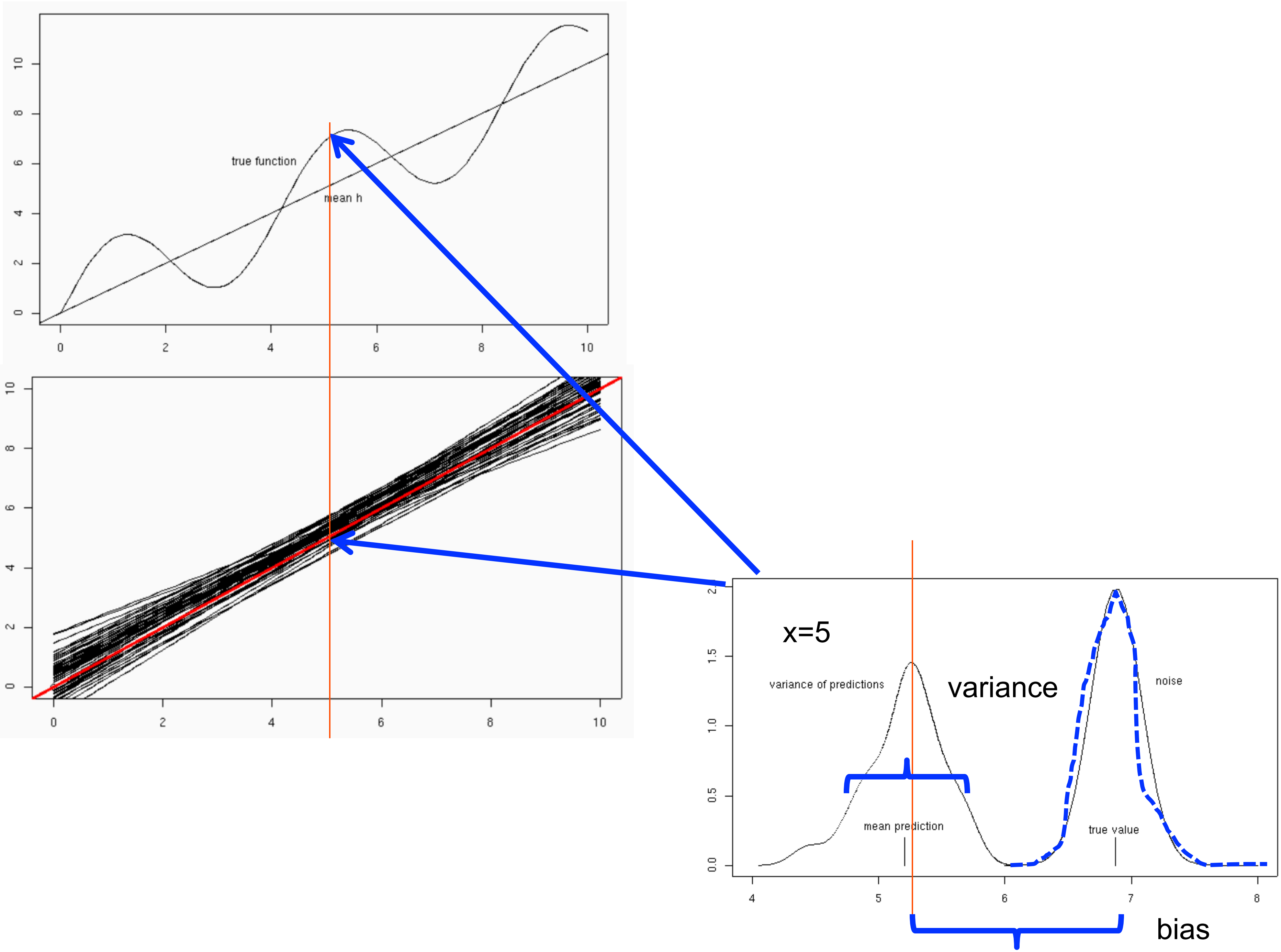
$$h \equiv E_D\{h_D(x)\}$$
$$\hat{y} = \hat{y}_D \equiv h_D(x)$$
$$f \equiv f(x)+\varepsilon$$

BIAS^2

Squared difference between <u>best possible</u> prediction for x, f(x), and our <u>"long-term" expectation for what the learner will do</u> if we averaged over many datasets D, $E_D[h_D(x)]$

VARIANCE

Squared difference btwn our long-term expectation for the learners performance, $E_D[h_D(x)]$, and what we <u>expect in a representative run on a dataset D</u> (hat y)


true function
mean h
x=5
variance of predictions
variance
noise
mean prediction
true value
bias

Bias-variance decomposition

- This is something real that you can (approximately) measure experimentally
  - if you have synthetic data
- Different learners and model classes have different *tradeoffs*
  - large bias/small variance: few features, highly regularized, highly pruned decision trees, large-k k-NN…
  - small bias/high variance: many features, less regularization, unpruned trees, small-k k-NN…

Bias-Variance Decomposition: Classification

A generalization of bias-variance decomposition to other loss functions

- "Arbitrary" real-valued loss $L(y,y')$
  But $L(y,y')=L(y',y)$, $L(y,y)=0$, and $L(y,y')!=0$ if $y!=y'$
- Define "optimal prediction":
  $y^* = argmin_{y'} L(t,y')$
- Define "main prediction of learner"
  $y_m=y_{m,D} = argmin_{y'} E_D\{L(y,y')\}$
- Define "bias of learner":
  $Bias(x)=L(y^*,y_m)$
- Define "variance of learner"
  $Var(x)=E_D[L(y_m,y)]$
- Define "noise for x":
  $N(x) = E_t[L(t,y^*)]$

Claim:
$E_{D,t}[L(t,y) = c_1N(x)+Bias(x)+c_2Var(x)$
where
$c_1=Pr_D[y=y^*] - 1$
$c_2=1$ if $y_m=y^*$, -1 else

$m=|D|$

For 0/1 loss, the *main prediction* is the most common class predicted by $h_D(x)$, weighting *h's* by Pr(D)

Domingos, A Unified Bias-Variance Decomposition and its Applications, ICML 2000

Bias and variance

- For **classification**, we can also decompose the error of a learned classifier into two terms: bias and variance
  - Bias: the class of models **can’t** fit the data.
  - **Fix**: a *more expressive* model class.
  - Variance: the class of models **could** fit the data, but doesn’t because it’s hard to fit.
  - **Fix**: a *less expressive* model class.

Bias-Variance Decomposition: Measuring

Bias-variance decomposition

- This is something real that you can (approximately) measure experimentally
  - if you have synthetic data
  - …or if you' re clever

  - You need to somehow approximate $E_D\{h_D(x)\}$
  - I.e., construct many variants of the dataset D

Background: “Bootstrap” sampling

- **Input**: dataset D
- **Output**: many variants of D: $D_1, \ldots, D_T$
- For t=1,….,T:
  - – $D_t = \{\ \}$
  - – For i=1…|D|:
    - Pick (**x**,y) uniformly at random from D (i.e., **with** replacement) and add it to D_t
    - Some examples never get picked (~37%)
    - Some are picked 2x, 3x, ….

Measuring Bias-Variance with "Bootstrap" sampling

- Create B bootstrap variants of D (approximate many draws of D)
- For each bootstrap dataset
  - T_b is the dataset; U_b are the "out of bag" examples
  - Train a hypothesis h_b on T_b
  - Test h_b on each x in U_b
- Now for each (**x**,y) example we have many predictions $h_1(x), h_2(x), \ldots.$ so we can estimate (ignoring noise)
  - **variance**: ordinary variance of $h_1(x), \ldots., h_n(x)$
  - **bias**: average$(h_1(x), \ldots, h_n(x))$ - y

Applying Bias-Variance Analysis

- By measuring the bias and variance on a problem, we can determine how to improve our model
  - If bias is high, we need to allow our model to be more complex
  - If variance is high, we need to reduce the complexity of the model
- Bias-variance analysis also suggests a way to reduce variance: *bagging* (later)

Bagging

Bootstrap Aggregation (Bagging)

- Use the **bootstrap** to create *B* variants of *D*
- Learn a classifier from **each variant**
- **Vote** the learned classifiers to predict on a test example

Bagging (bootstrap aggregation)

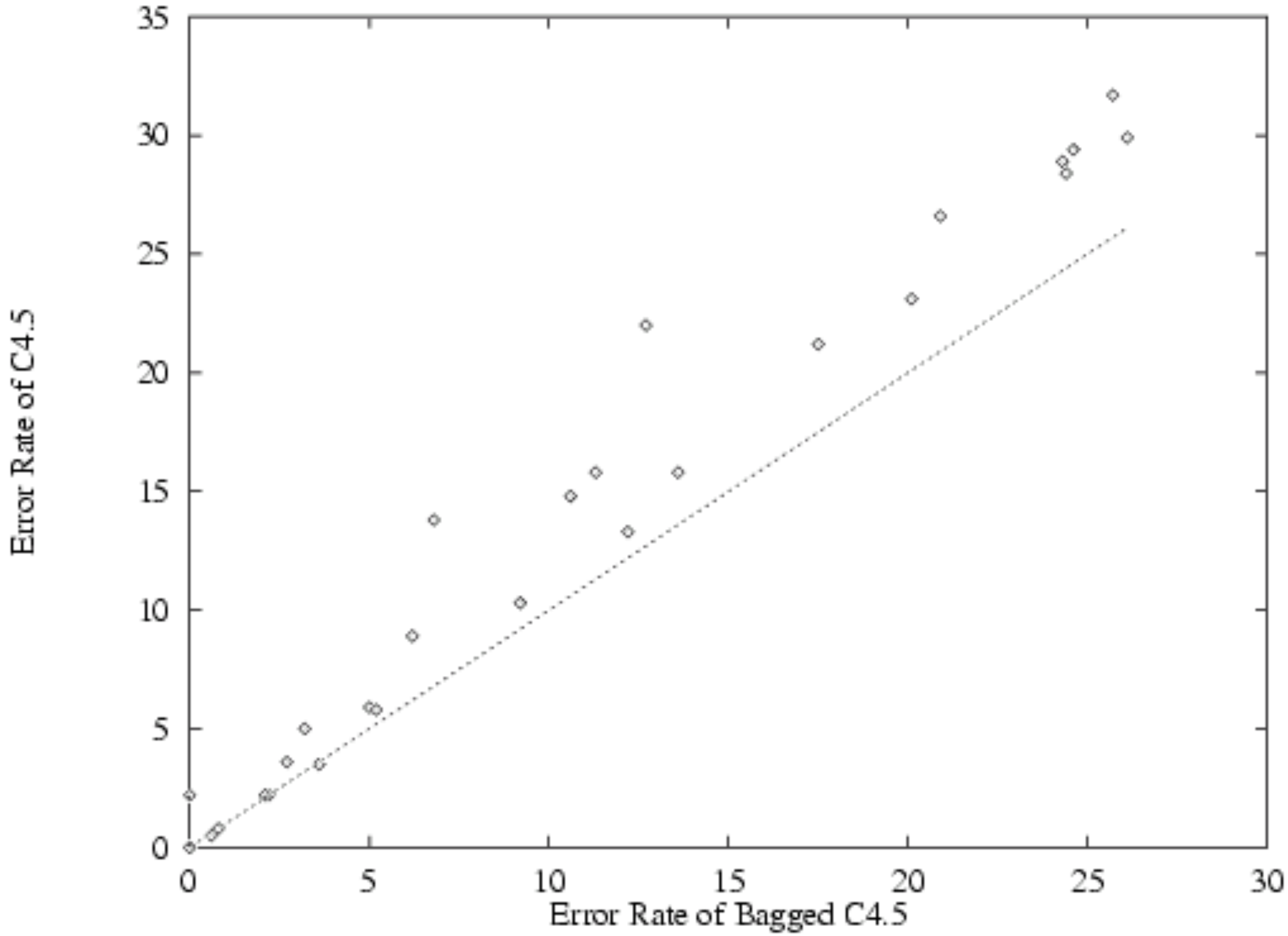
- Breaking it down:
  - input: dataset D and YFCL
  - output: a classifier $h_{D\text{-}BAG}$
  - use bootstrap to construct variants $D_1,\ldots,D_T$
  - for $t=1,\ldots,T$: train YFCL on D_t to get h_t
  - to classify x with $h_{D\text{-}BAG}$
    - classify x with $h_1,\ldots,h_T$ and predict the most frequently predicted class for x (majority vote)

Note that you can use *any* learner you like!

You can also test h_t on the "out of bag" examples

Experiments

Freund and Schapire

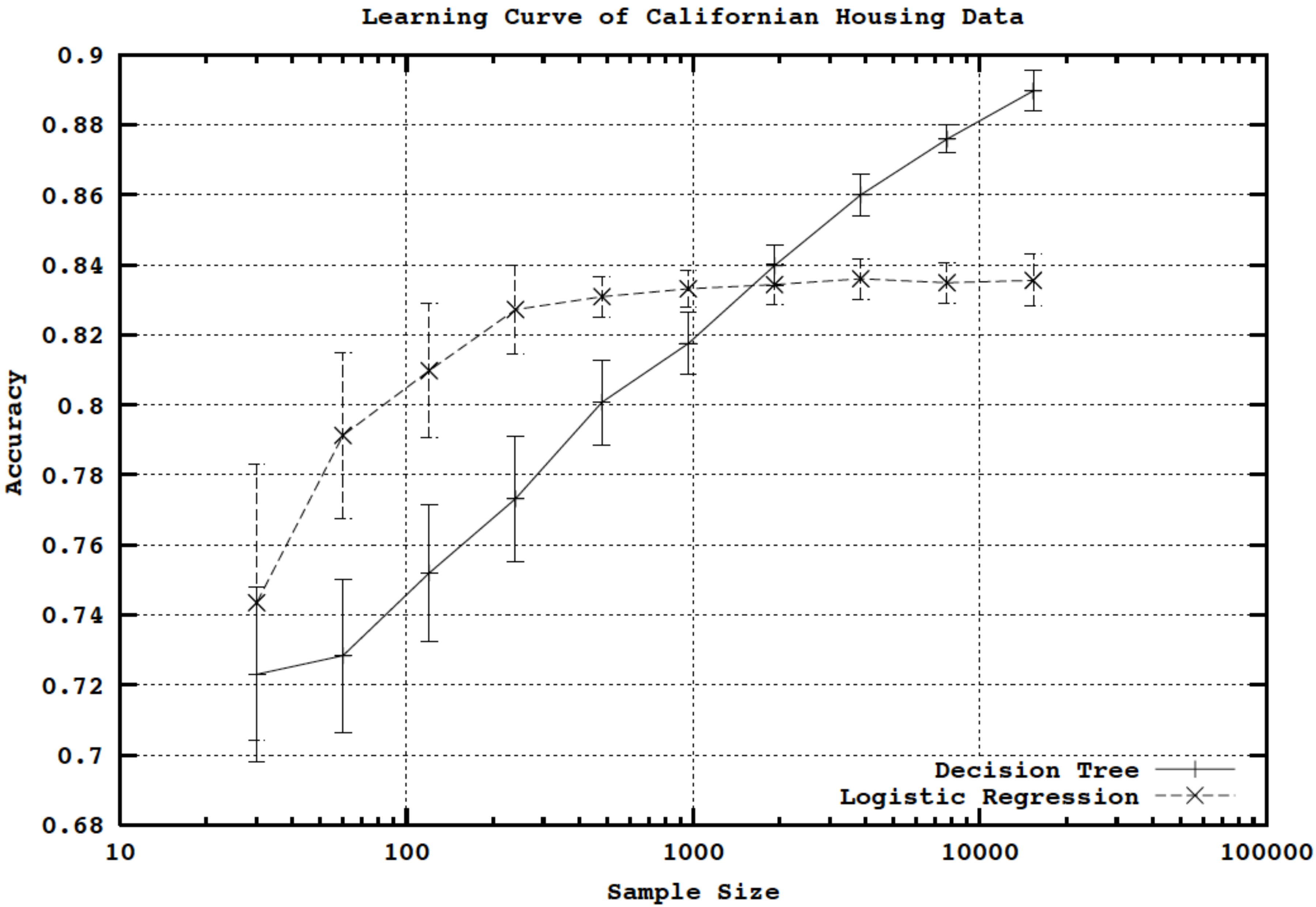


Journal of Machine Learning Research 4 (2003) 211-255 Submitted 12/01; Revised 2/03; Published 6/03

Tree Induction vs. Logistic Regression: A Learning-Curve Analysis

Bagged, minimally pruned decision trees

Claudia Perlich CPERLICH@STERN.NYU.EDU
Foster Provost FPROVOST@STERN.NYU.EDU
Jeffrey S. Simonoff JSIMONOF@STERN.NYU.EDU
Leonard N. Stern School of Business
New York University
44 West 4th Street
New York, NY 10012



Learning Curve of Californian Housing Data
Accuracy
0.9
0.88
0.86
0.84
0.82
0.8
0.78
0.76
0.74
0.72
0.7
0.68
10
100
1000
10000
100000
Sample Size
Decision Tree
Logistic Regression

Generally, bagged decision trees outperform the linear classifier eventually if the data is large enough and clean enough.

Data set	Winner AUR	Winner Acc	Max-AUR	Result
Nurse	none	none	1	Indistinguishable
Mushrooms	none	none	1	Indistinguishable
Optdigit	none	none	0.99	Indistinguishable
Letter–V	C4	C4	0.99	C4 dominates
Letter–A	C4	C4	0.99	C4 crosses
Intrusion	C4	C4	0.99	C4 dominates
DNA	C4	C4	0.99	C4 dominates
Covertype	C4	C4	0.99	C4 crosses
Telecom	C4	C4	0.98	C4 dominates
Pendigit	C4	C4	0.98	C4 dominates
Pageblock	C4	C4	0.98	C4 crosses
CarEval	none	C4	0.98	C4 crosses
Spam	C4	C4	0.97	C4 dominates
Chess	C4	C4	0.95	C4 dominates
CalHous	C4	C4	0.95	C4 crosses
Ailerons	none	C4	0.95	C4 crosses
Firm	LR	LR	0.93	LR crosses
Credit	C4	C4	0.93	C4 dominates
Adult	LR	C4	0.9	Mixed
Connects	C4	none	0.87	C4 crosses
Move	C4	C4	0.85	C4 dominates
Downsize	C4	C4	0.85	C4 crosses
Coding	C4	C4	0.85	C4 crosses
German	LR	LR	0.8	LR dominates
Diabetes	LR	LR	0.8	LR dominates
Bookbinder	LR	LR	0.8	LR crosses
Bacteria	none	C4	0.79	C4 crosses
Yeast	*none*	*none*	*0.78*	*Indistinguishable*
Patent	C4	C4	0.75	C4 crosses
Contra	*none*	*none*	*0.73*	*Indistinguishable*
IntShop	LR	LR	0.7	LR crosses
IntCensor	LR	LR	0.7	LR dominates
Insurance	*none*	*none*	*0.7*	*Indistinguishable*
IntPriv	LR	none	0.66	LR crosses
Mailing	LR	none	0.61	LR dominates
Abalone	LR	LR	0.56	LR dominates

Bagging (bootstrap aggregation)

- Experimentally:
  - especially with minimal pruning: decision trees have low *bias* but high *variance*.
  - bagging usually improves performance for decision trees and similar methods
  - It reduces *variance* without increasing the bias (much).

More detail on bias-variance and bagging for classification

Thanks Tom Dietterich MLSS 2014

A generalization of bias-variance decomposition to other loss functions

- "Arbitrary" real-valued loss *L(y,y')*
  But L(y,y')=L(y' ,y), L(y,y)=0, and L(y,y')!=0 if y!=y'
- Define "optimal prediction":
  $y^* = \mathrm{argmin}_{y'} L(t,y')$
- Define "main prediction of learner"
  $y_m = y_{m,D} = \mathrm{argmin}_{y'} E_D\{L(y,y')\}$

$m=|D|$

- Define "bias of learner":
  $Bias(x)=L(y^*,y_m)$
- Define "variance of learner"
  $Var(x)=E_D[L(y_m,y)]$
- Define "noise for x":
  $N(x) = E_t[L(t,y^*)]$

Claim:
$E_{D,t}[L(t,y) = c_1 N(x)+Bias(x)+c_2 Var(x)$
where
$c_1=Pr_D[y=y^*] - 1$
$c_2=1$ if $y_m=y^*$, -1 else

For 0/1 loss, the *main prediction* is the most common class predicted by $h_D(x)$, weighting *h's* by Pr(D)

Domingos, A Unified Bias-Variance Decomposition and its Applications, ICML 2000

More detail on Domingos's model

- *Noisy channel*: $y_i = noise(f(x_i))$
  - $f(x_i)$ is true label of x_i
  - Noise *noise(.)* may change $y \rightarrow y'$
- $h=h_D$ is learned hypothesis
  - from $D=\{(x_1,y_1),\ldots(x_m,y_m)\}$
- for test case (x^*,y^*), and predicted label $h(x^*)$, *loss* is $L(h(x^*),y^*)$
  - For instance, $L(h(x^*),y^*) = 1$ if error, else 0

More detail on Domingos's model

- We want to decompose $E_{D,P}\{L(h(x^*),y^*)\}$ where m is size of D, $(x^*,y^*)\sim P$
- *Main prediction of learner* is $y_m(x^*)$
  - $y_m(x^*) = \text{argmin}_{y'}\ E_{D,P}\{L(h(x^*),y')\}$
  - $y_m(x^*)$ = "most common" $h_D(x^*)$ among all possible *D*'s, weighted by Pr(*D*)
- *Bias* is $B(x^*) = L(y_m(x^*), f(x^*))$
- *Variance* is $V(x^*) = E_{D,P}\{L(h_D(x^*), y_m(x^*))$
- *Noise* is $N(x^*) = L(y^*, f(x^*))$

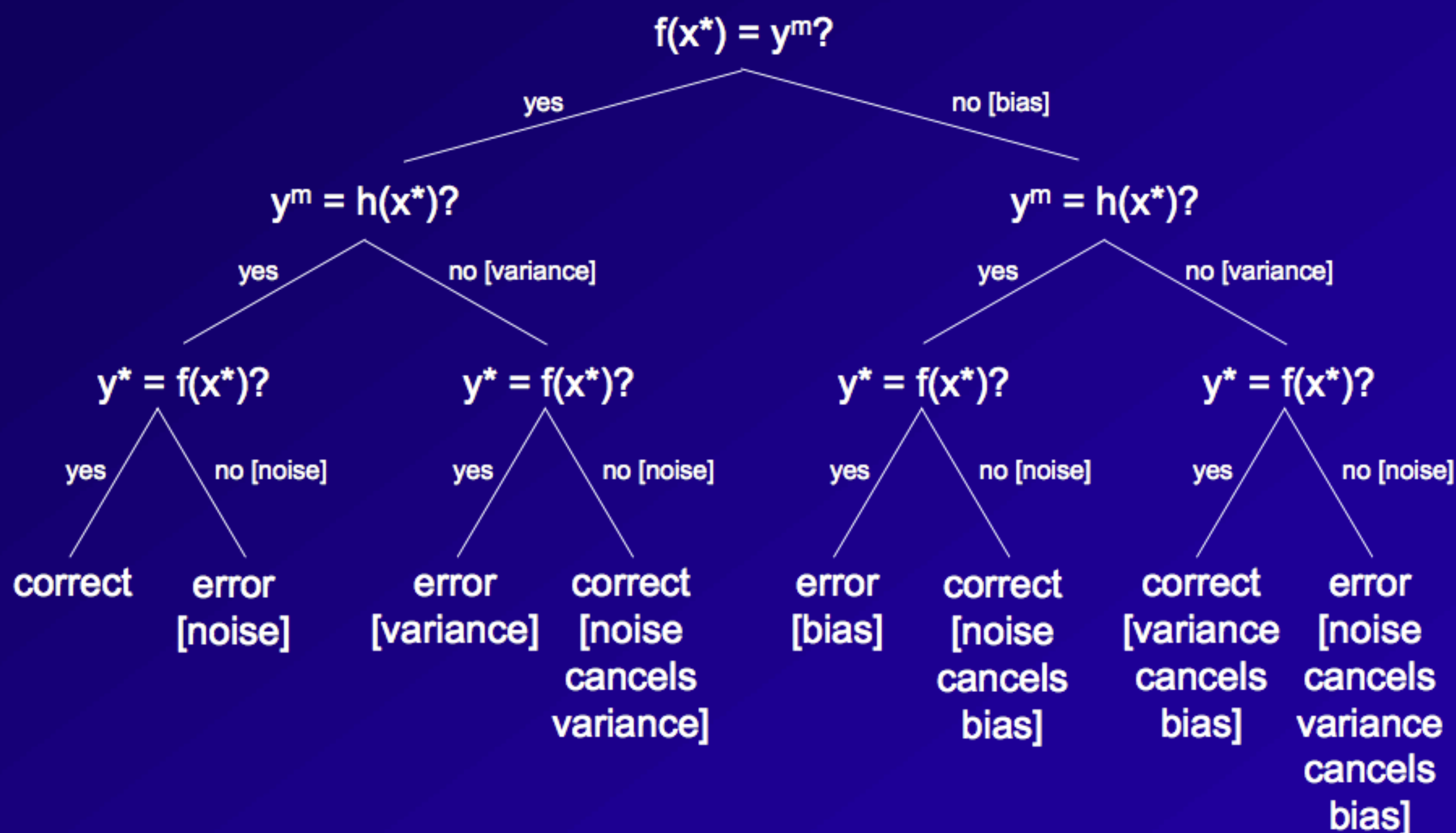
More detail on Domingos' s model

- We want to decompose $E_{D,P}\{L(h(x^*),y^*)\}$
- *Main prediction of learner* is $y_m(x^*)$
  - "most common" $h_D(x^*)$ over *D's* for 0/1 loss
- *Bias* is $B(x^*) = L(y_m(x^*)\ , f(x^*))$
  - main prediction vs true label
- *Variance* is $V(x^*) = E_{D,P}\{L(h_D(x^*)\ , y_m(x^*)\ )$
  - this hypothesis vs main prediction
- *Noise* is $N(x^*)= L(y^*, f(x^*))$
  - true label vs observed label

More detail on Domingos' s model

- We will decompose $E_{D,P}\{L(h(x^*),y^*)\}$ into
  - *Bias* is $B(x^*) = L(y_m(x^*) , f(x^*))$
    - main prediction vs true label
    - this is 0/1, *not* a random variable
  - *Variance* is $V(x^*) = E_{D,P}\{L(h_D(x^*) , y_m(x^*))$
    - this hypothesis vs main prediction
  - *Noise* is $N(x^*)= L(y^*, f(x^*))$
    - true label vs observed label

Case analysis of error



Analysis of error: unbiased case

- Let $P(y^* \neq f(x^*)) = N(x^*) = \tau$
- Let $P(y^m \neq h(x^*)) = V(x^*) = \sigma$
- If $(f(x^*) = y^m)$, then we suffer a loss if exactly one of these events occurs:

$$L(h(x^*), y^*) = \tau(1-\sigma) + \sigma(1-\tau)$$
$$= \tau + \sigma - 2\tau\sigma$$
$$= N(x^*) + V(x^*) - 2\, N(x^*)\, V(x^*)$$

Variance but no noise

Main prediction is correct

Noise but no variance

Analysis of error: biased case

- Let $P(y^* \neq f(x^*)) = N(x^*) = \tau$
- Let $P(y^m \neq h(x^*)) = V(x^*) = \sigma$
- If $(f(x^*) \neq y^m)$, then we suffer a loss if either both or neither of these events occurs:

$$L(h(x^*), y^*) = \tau\sigma + (1-\sigma)(1-\tau)$$
$$= 1 - (\tau + \sigma - 2\tau\sigma)$$
$$= B(x^*) - [N(x^*) + V(x^*) - 2\,N(x^*)\,V(x^*)]$$

No noise, no variance

Main prediction is wrong

Noise and variance

Analysis of error: overall

$E[\, L(h(x^*), y^*)\,] =$

if $B(x^*) = 1$: $B(x^*) - [N(x^*) + V(x^*) - 2\, N(x^*)\, V(x^*)]$

if $B(x^*) = 0$: $B(x^*) + [N(x^*) + V(x^*) - 2\, N(x^*)\, V(x^*)]$

Hopefully we'll be in this case more often, if we've chosen a good classifier

Interaction terms are usually small

Analysis of error: without noise

which is hard to estimate anyway

$$E[\, L(h(x^*), y^*)\,] =$$

$$\text{if } B(x^*) = 1: \quad B(x^*) - V(x^*)$$

$$\text{if } B(x^*) = 0: \quad B(x^*) + V(x^*)$$

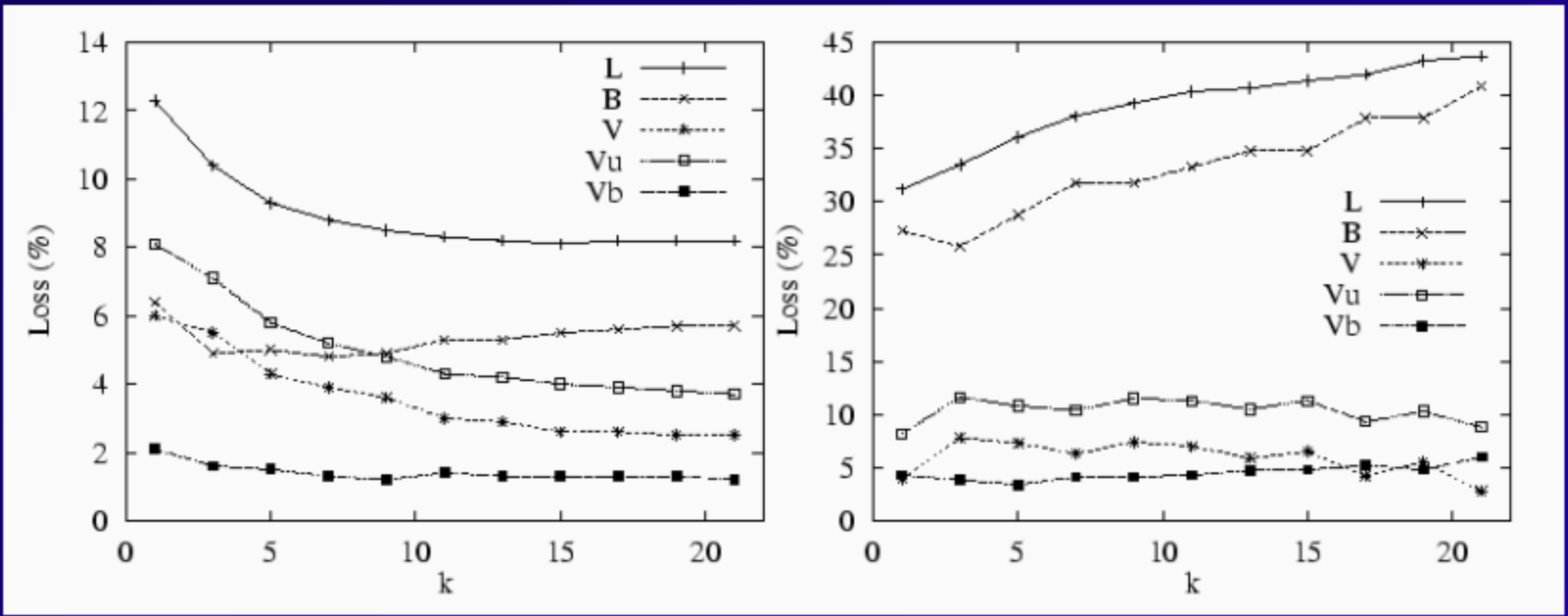
Vb

Vu

As with regression, we can experimentally approximately measure bias and variance with bootstrap replicates

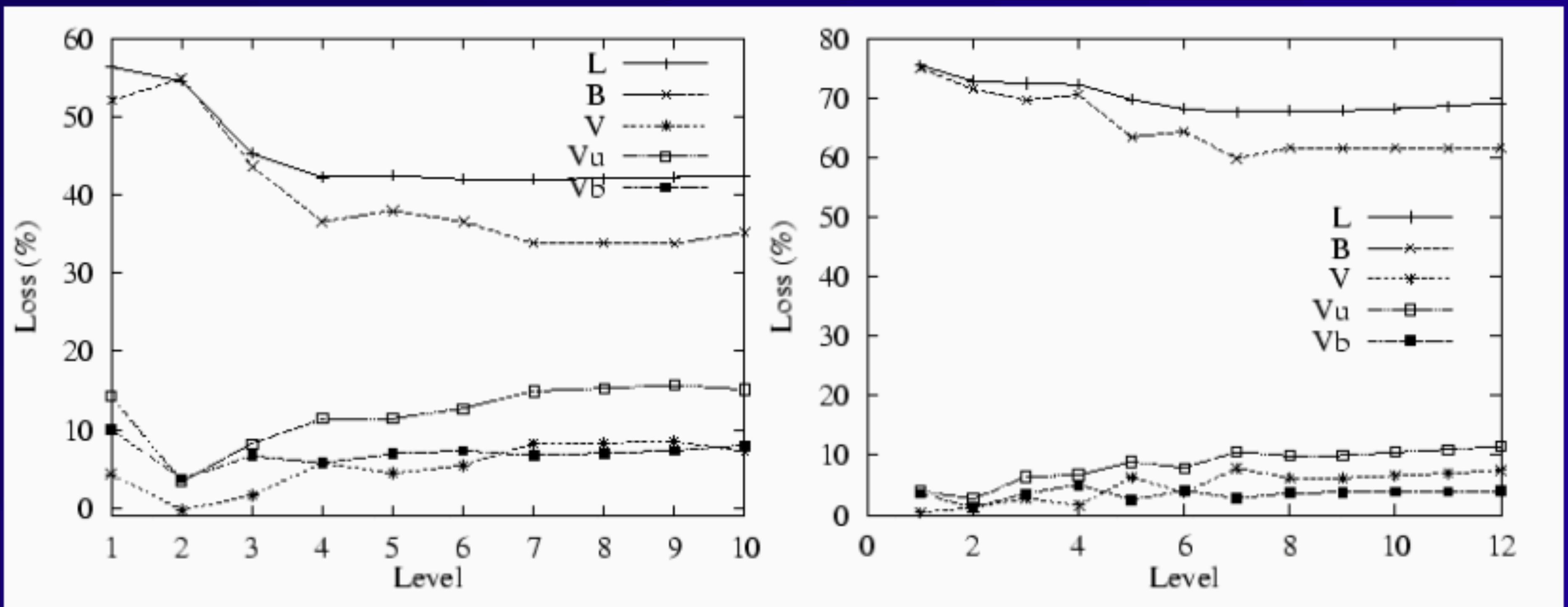
Typically break variance down into *biased variance, Vb,* and *unbiased variance, Vu.*

K-NN Experiments



- Chess (left): Increasing K primarily reduces Vu
- Audiology (right): Increasing K primarily increases B.

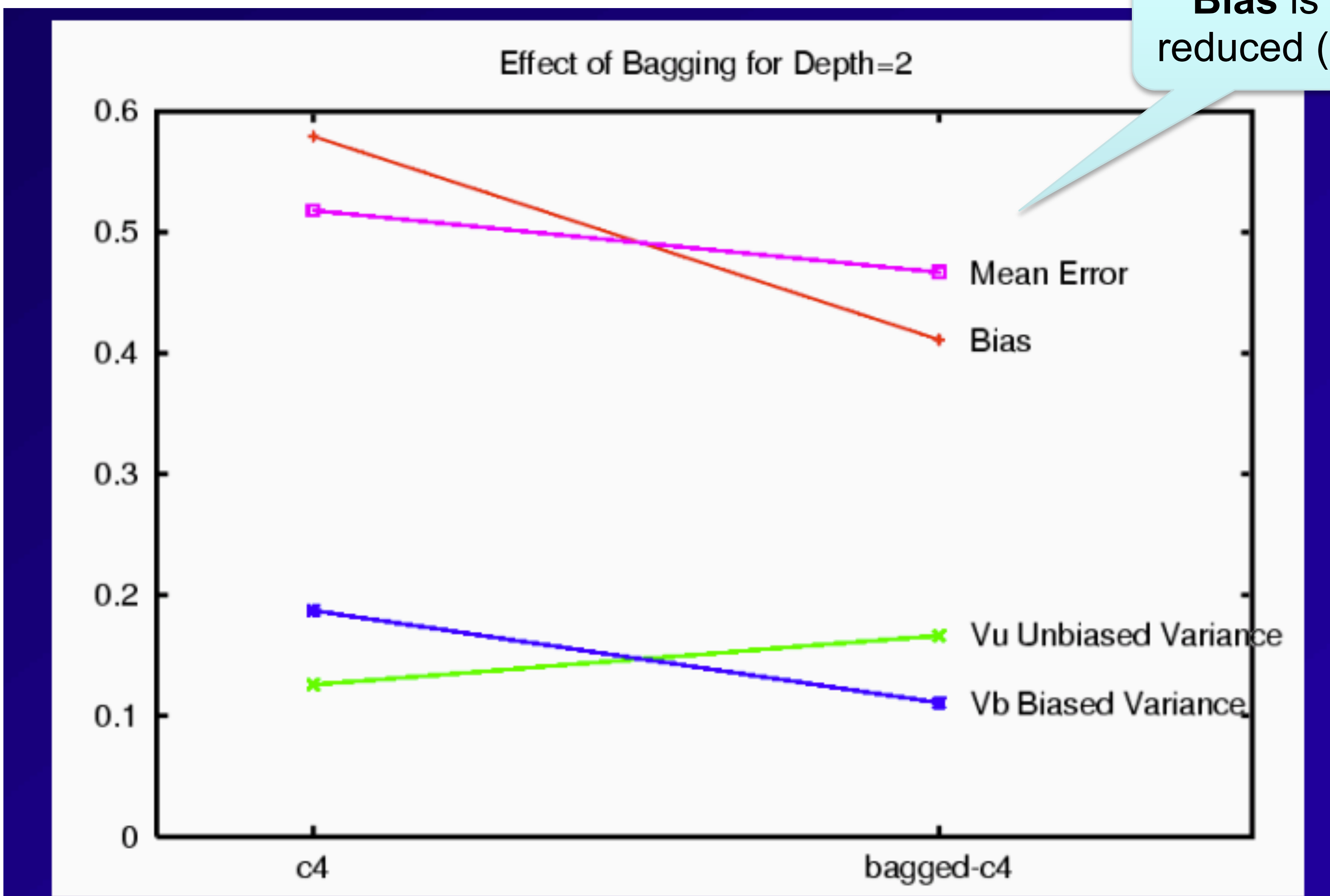
Tree Experiments



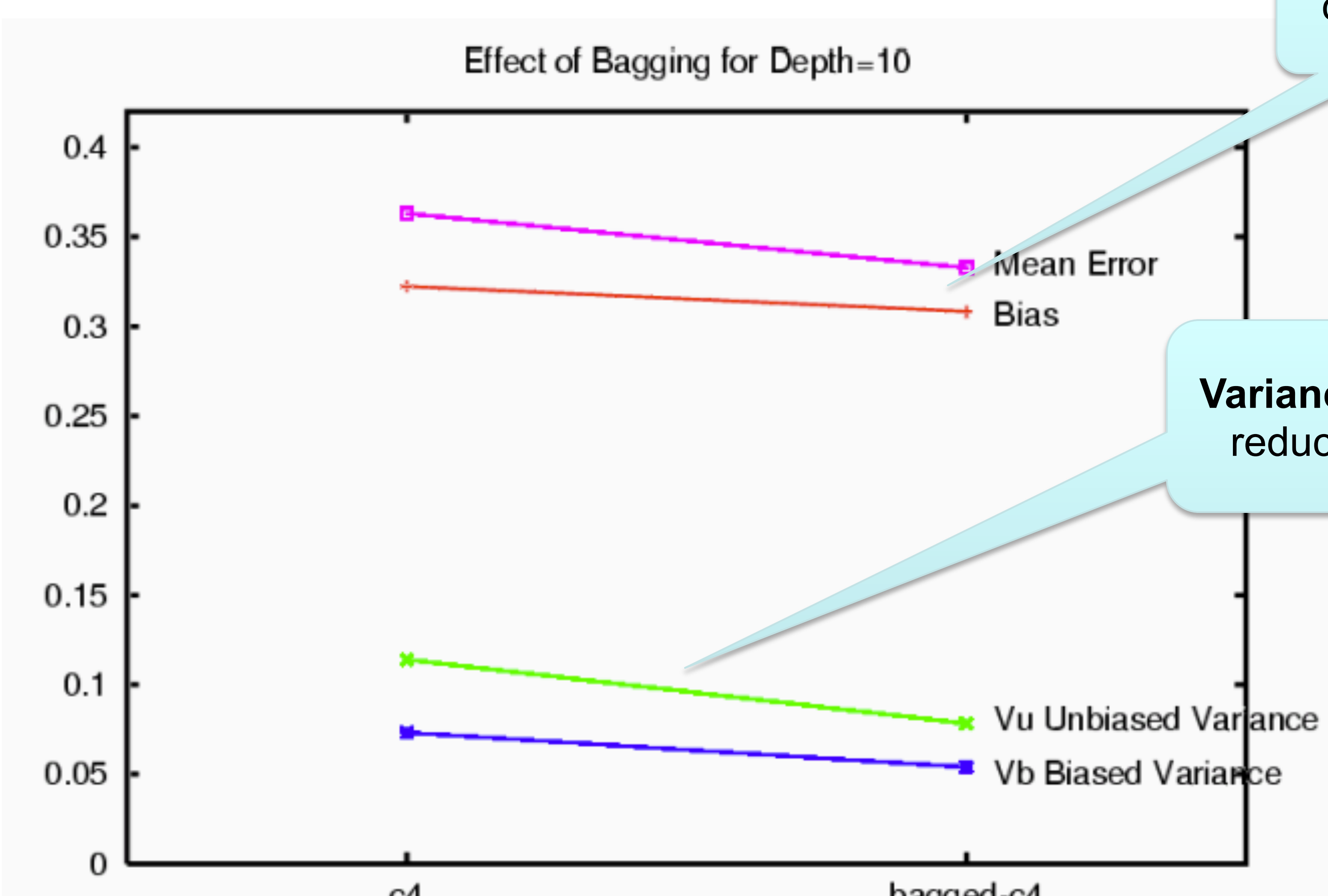
- Glass (left), Primary tumor (right): deeper trees have lower B, higher Vu

Tree "stump" experiments (depth 2)

Bias is reduced (!)



Large tree experiments (depth 10)



Bias is not changed much

Variance is reduced