Lecture 5

Regression Modelling And Information Theory

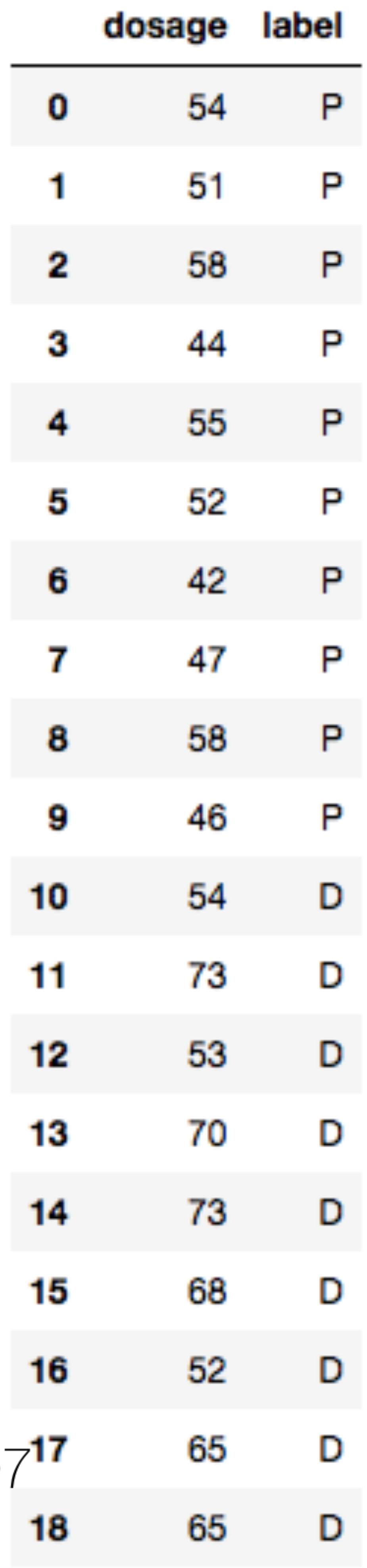
Last Time:

- Small World vs Big World
- MLE and Sampling
- Gaussian MLE
- Fitting without Noise
- What is noise?
- Fitting with Noise
- Test sets

Today

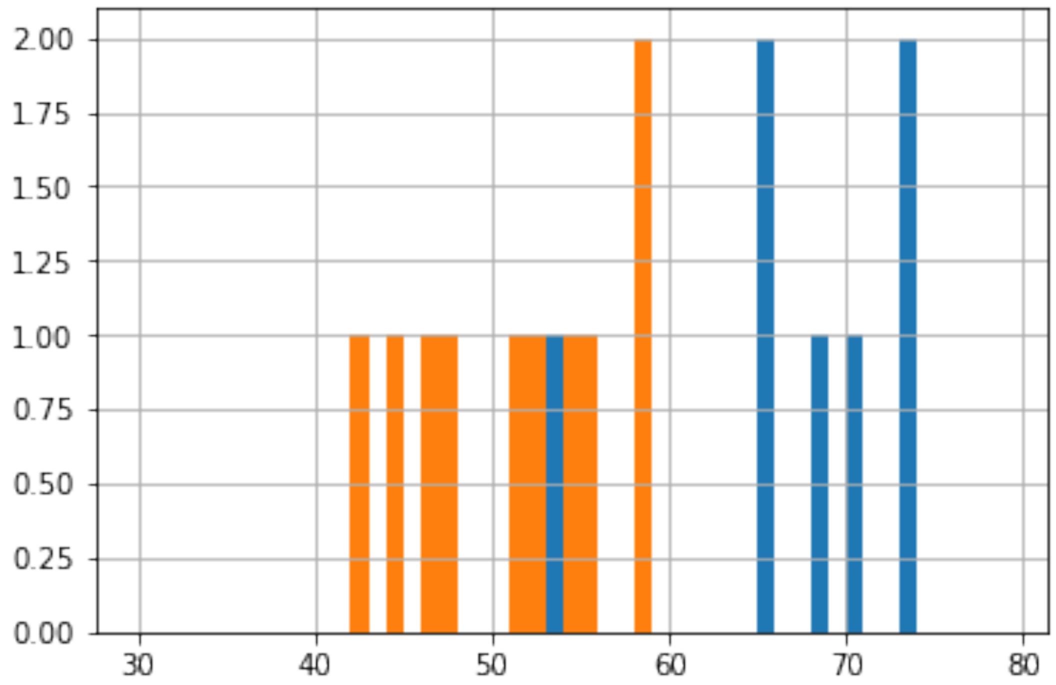
- More on significance
- Test Sets
- Validation and X-validation
- Regularization
- The KL Divergence and Deviance
- In-sample penalties: the AIC

Dose vs Placebo

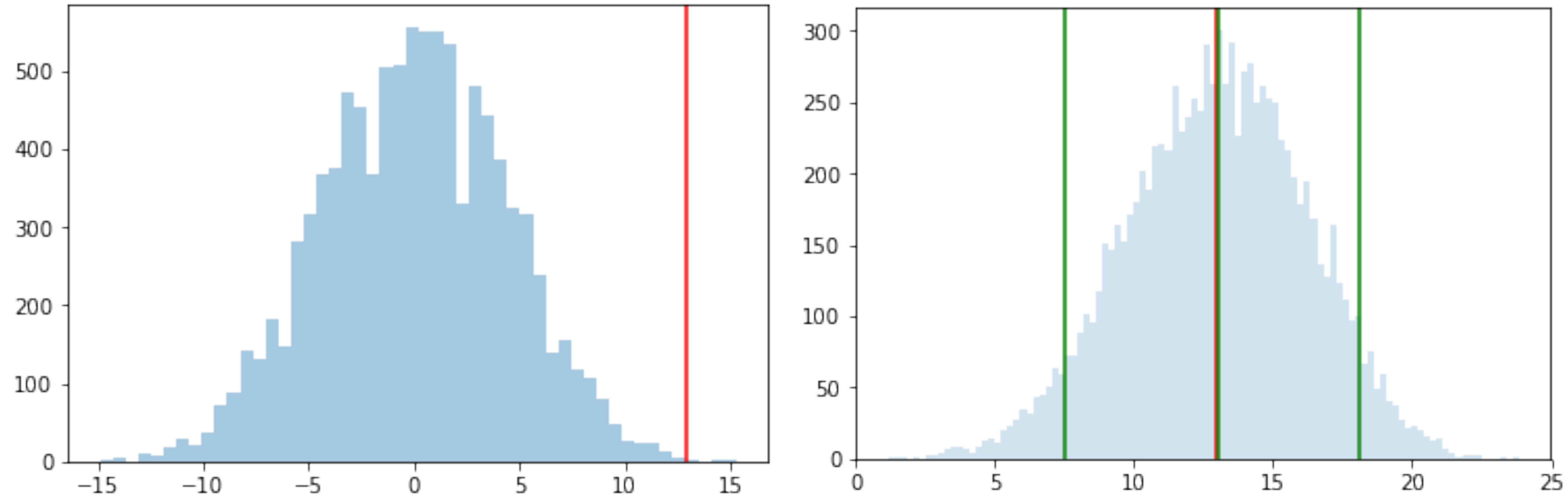


	dosage	label
0	54	P
1	51	P
2	58	P
3	44	P
4	55	P
5	52	P
6	42	P
7	47	P
8	58	P
9	46	P
10	54	D
11	73	D
12	53	D
13	70	D
14	73	D
15	68	D
16	52	D
17	65	D
18	65	D

Actual mean effect is about 13.



Significance vs Size of Effect



Left, permute all labels. Right, sample with replacement within groups.

HYPOTHESIS SPACES

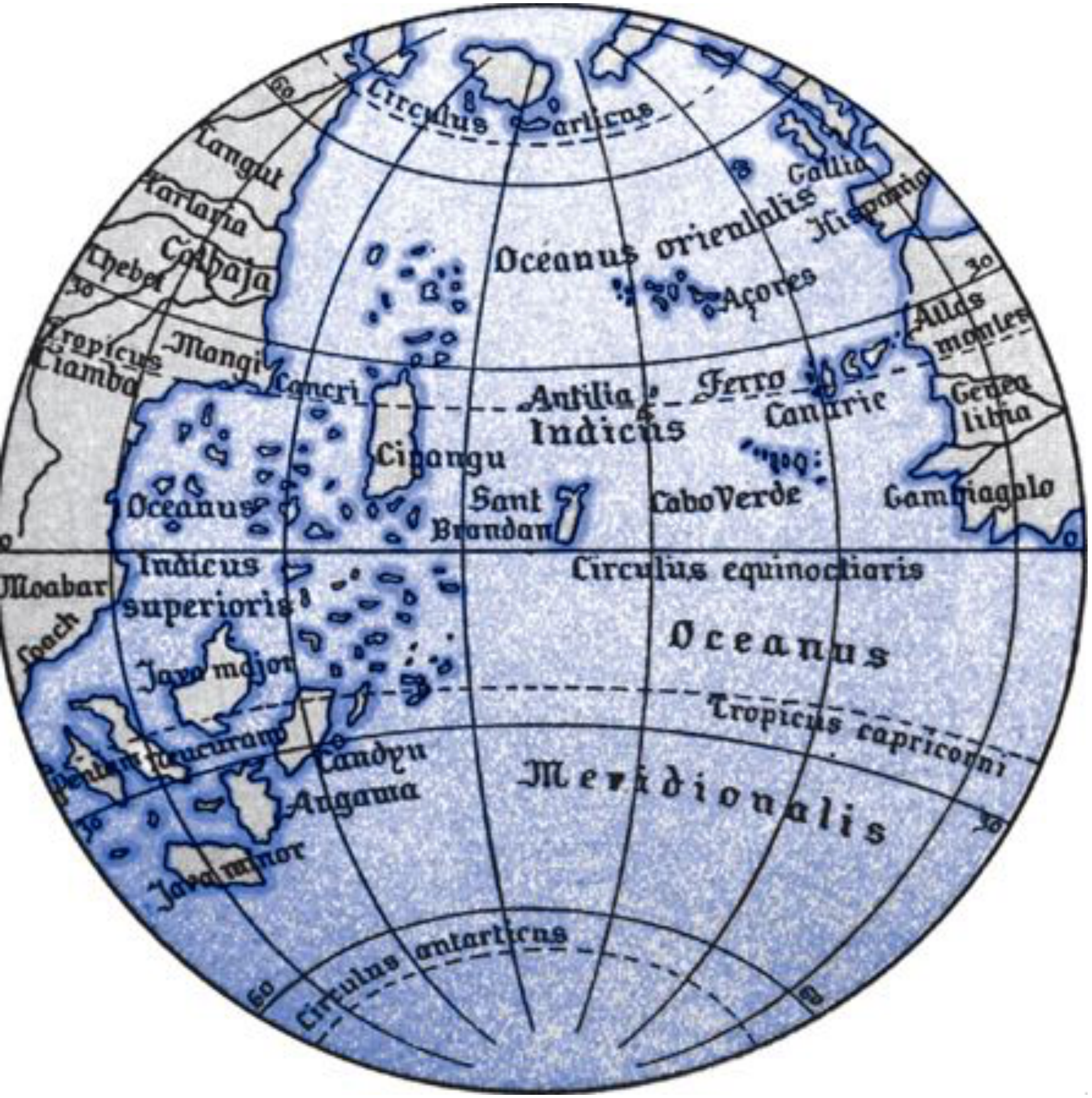
A polynomial looks so:

$$h(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2 + \ldots + \theta_n x^n = \sum_{i=0}^{n} \theta_i x^i$$

All polynomials of a degree or complexity d constitute a hypothesis space.

$$\mathcal{H}_1 : h_1(x) = \theta_0 + \theta_1 x$$

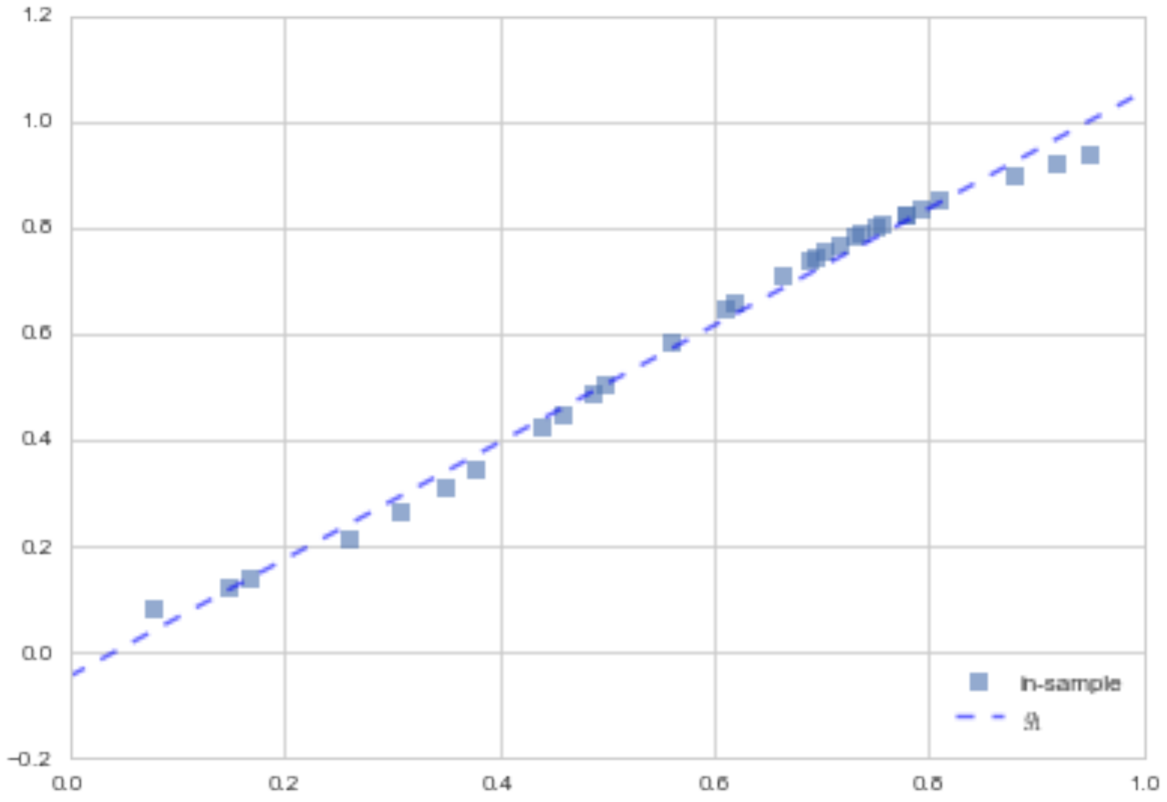
SMALL World vs BIG World

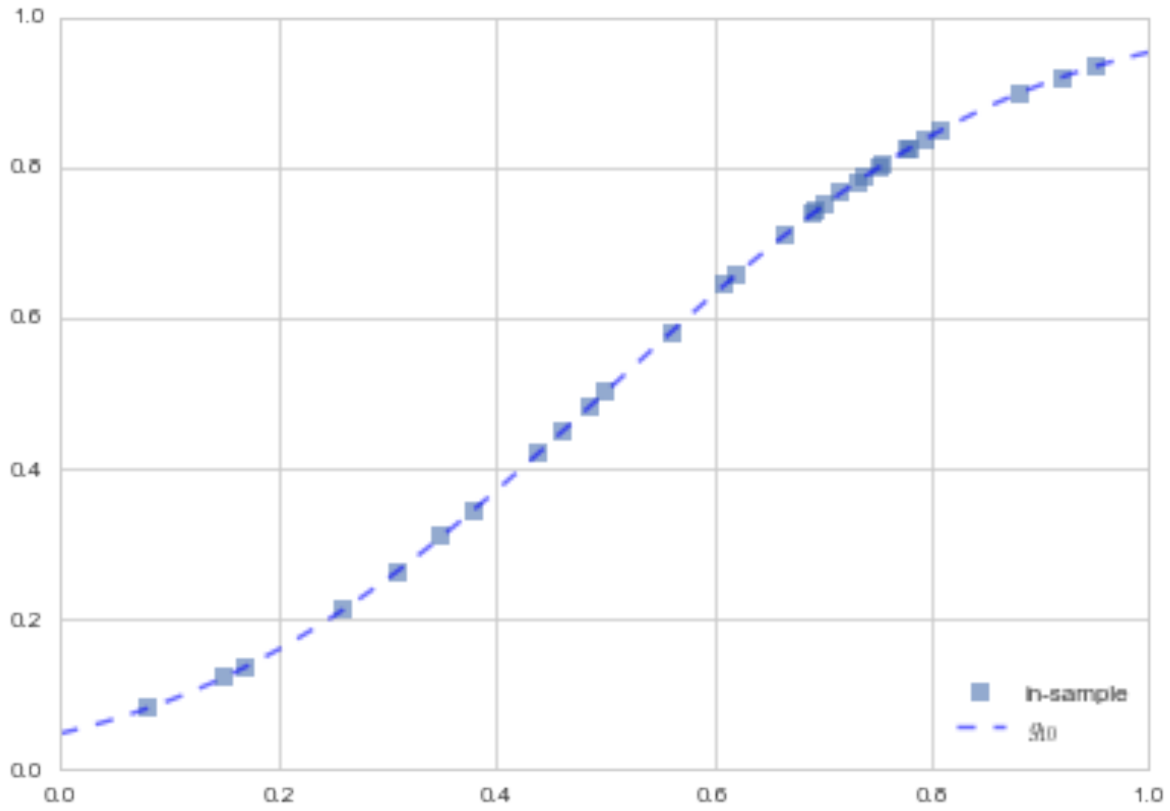


- *Small World* answers the question: given a model class (i.e. a Hypothesis space, whats the best model in it). It involves parameters. Its model checking.
- *BIG World* compares model spaces. Its model comparison with or without "hyperparameters".

Without Noise...

30 points of data. Which fit is better? Line in $\mathcal{H}_1$ or curve in $\mathcal{H}_{20}$?

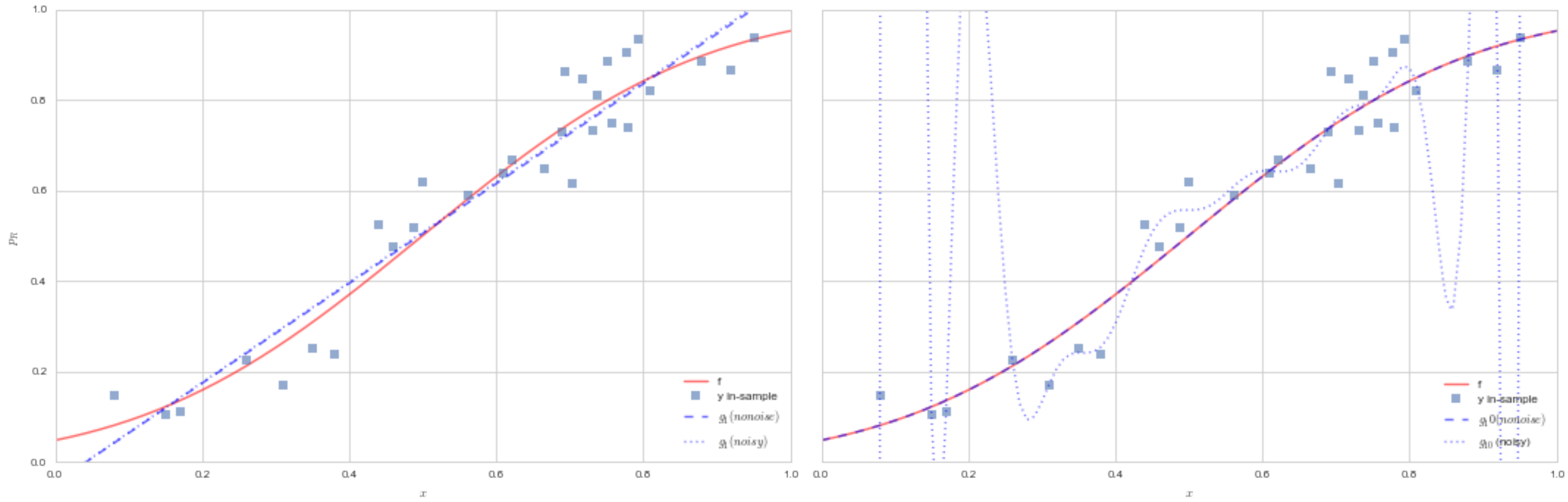




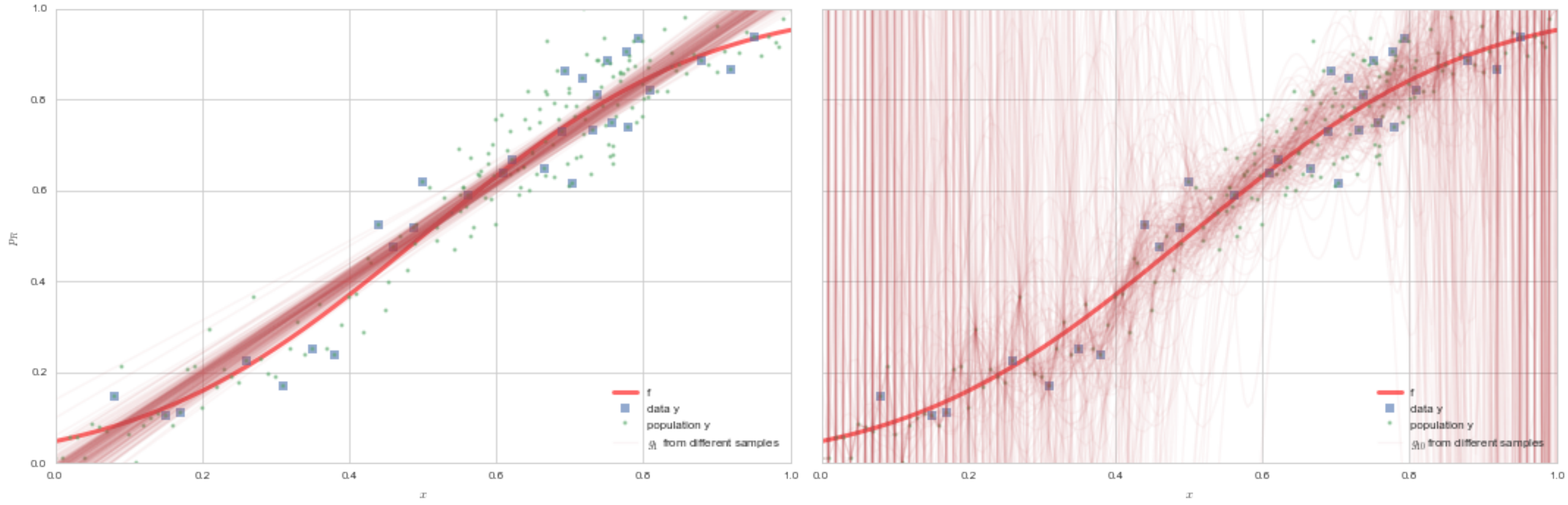
THE REAL WORLD HAS NOISE

Which fit is better now?

The line or the curve?



UNDERFITTING (Bias)
vs OVERFITTING (Variance)



Every model has Bias and Variance

$$R_{out}(h) = E_{p(x)}[(h(x) - y)^2] = \int dx p(x)(h(x) - f(x) - \epsilon)^2.$$

Fit hypothesis $h = g_{\mathcal{D}}$, where $\mathcal{D}$ is our training sample.

Define:

$$\langle R \rangle = \int dy dx \, p(x, y)(h(x) - y)^2 = \int dy dx p(y \mid x)p(x)(h(x) - y)^2.$$

$$\langle R \rangle = E_{\mathcal{D}}[R_{out}(g_{\mathcal{D}})] = E_{\mathcal{D}}E_{p(x)}[(g_{\mathcal{D}}(x) - f(x) - \epsilon)^2]$$

$$\bar{g} = E_{\mathcal{D}}[g_{\mathcal{D}}] = (1/M)\sum_{\mathcal{D}} g_{\mathcal{D}}$$

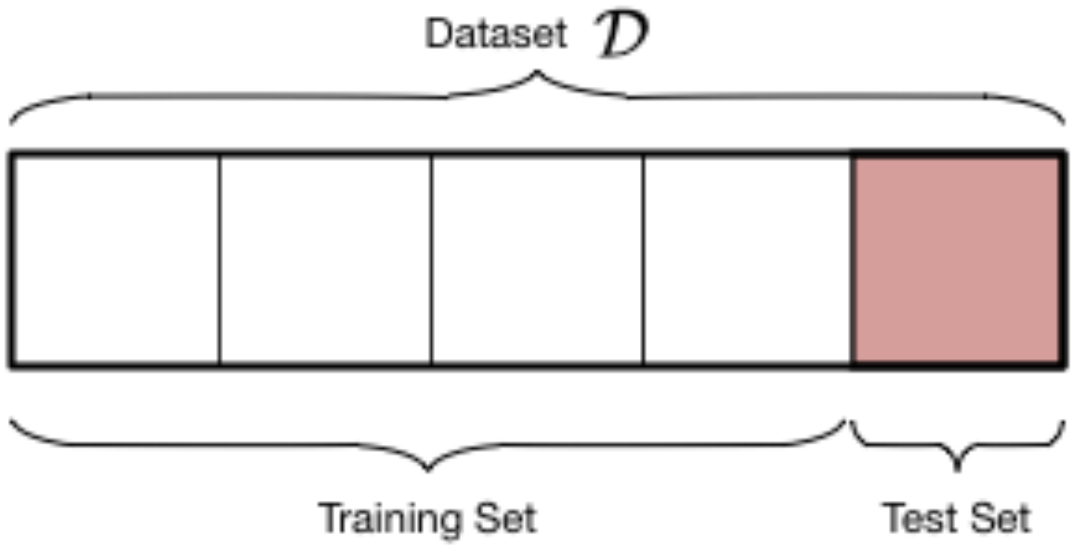
Then,

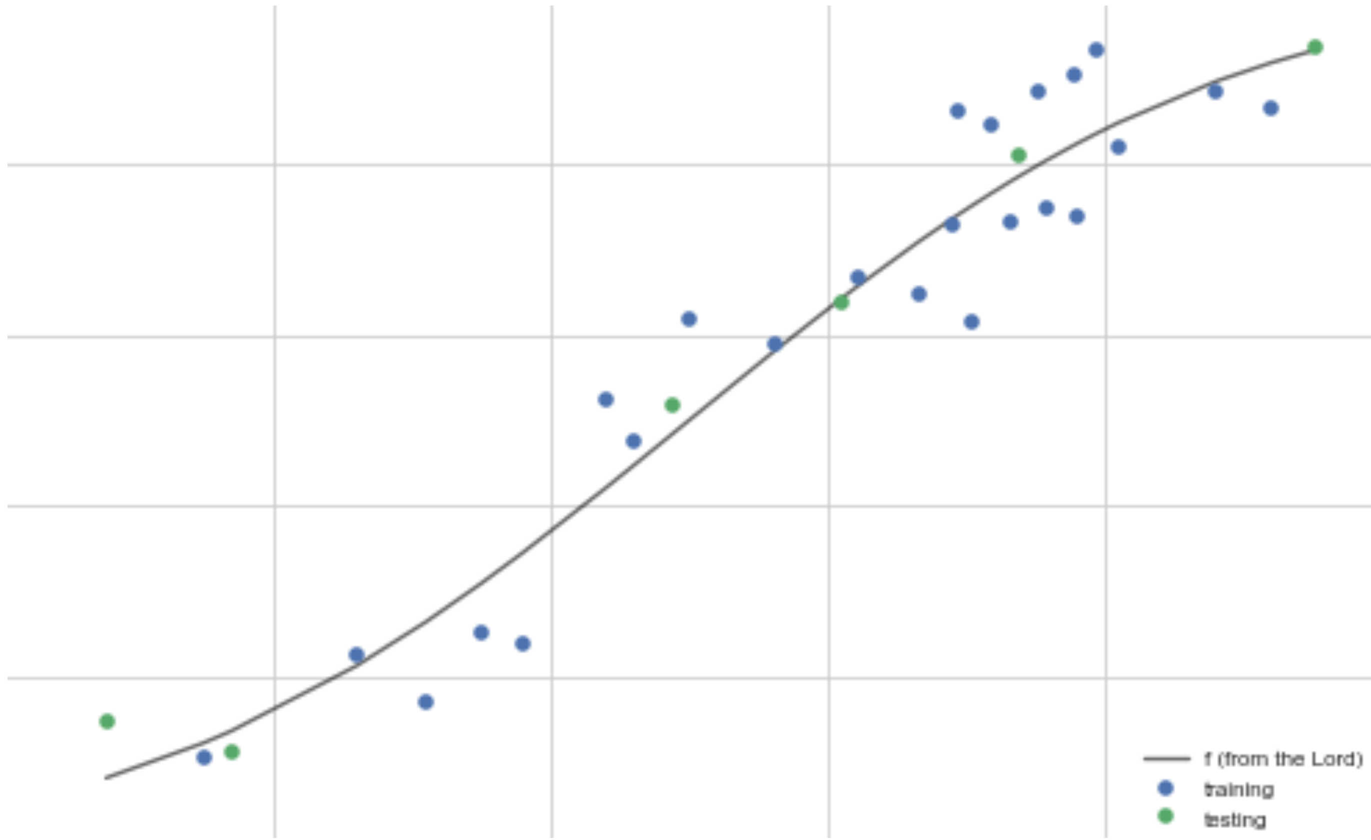
$$\langle R \rangle = E_{p(x)}[E_{\mathcal{D}}[(g_{\mathcal{D}} - \bar{g})^2]] + E_{p(x)}[(f - \bar{g})^2] + \sigma^2$$

This is the bias variance decomposition for regression.

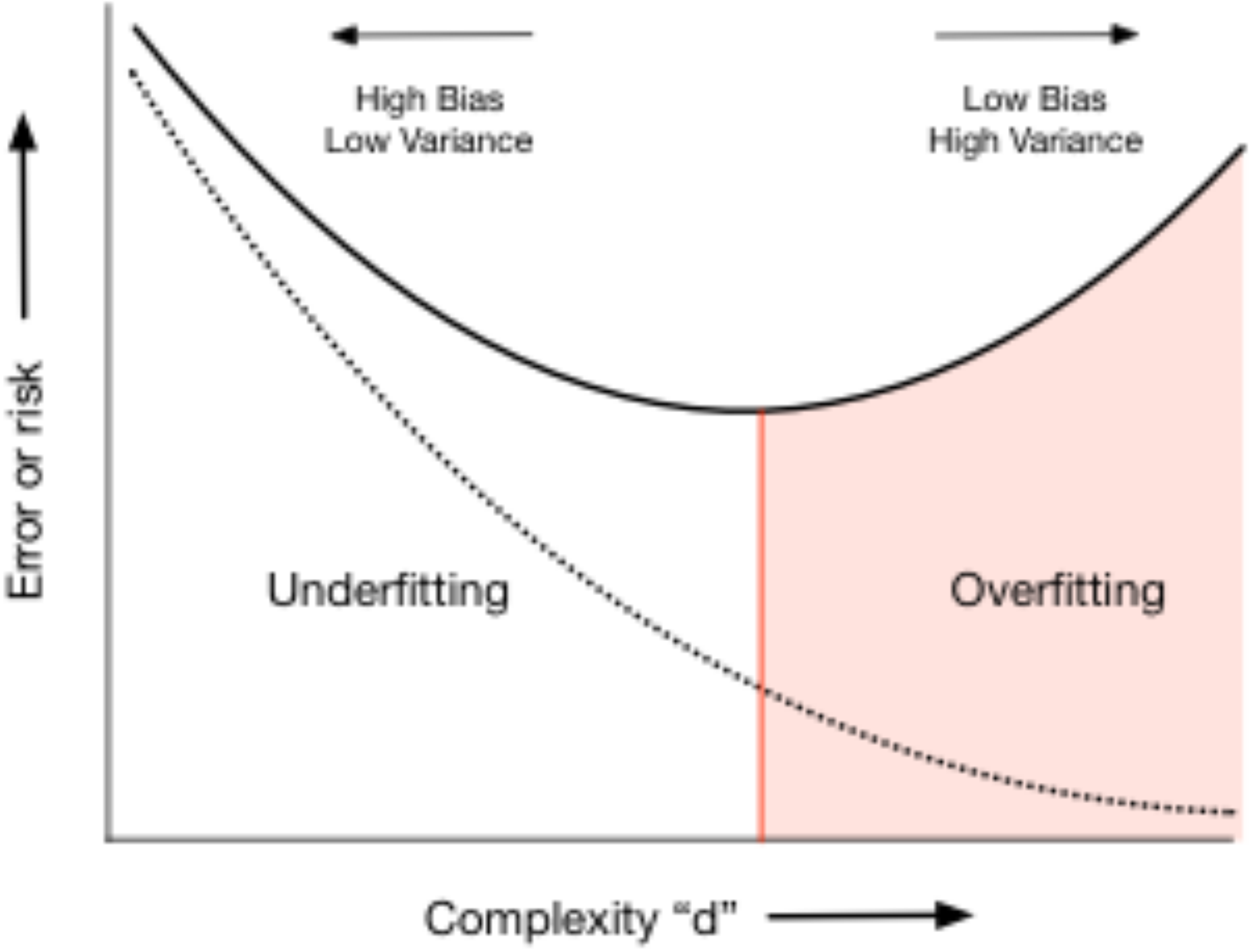
- first term is **variance**, squared error of the various fit g's from the average g, the hairiness.
- second term is **bias**, how far the average g is from the original f this data came from.
- third term is the **stochastic noise**, minimum error that this model will always have.

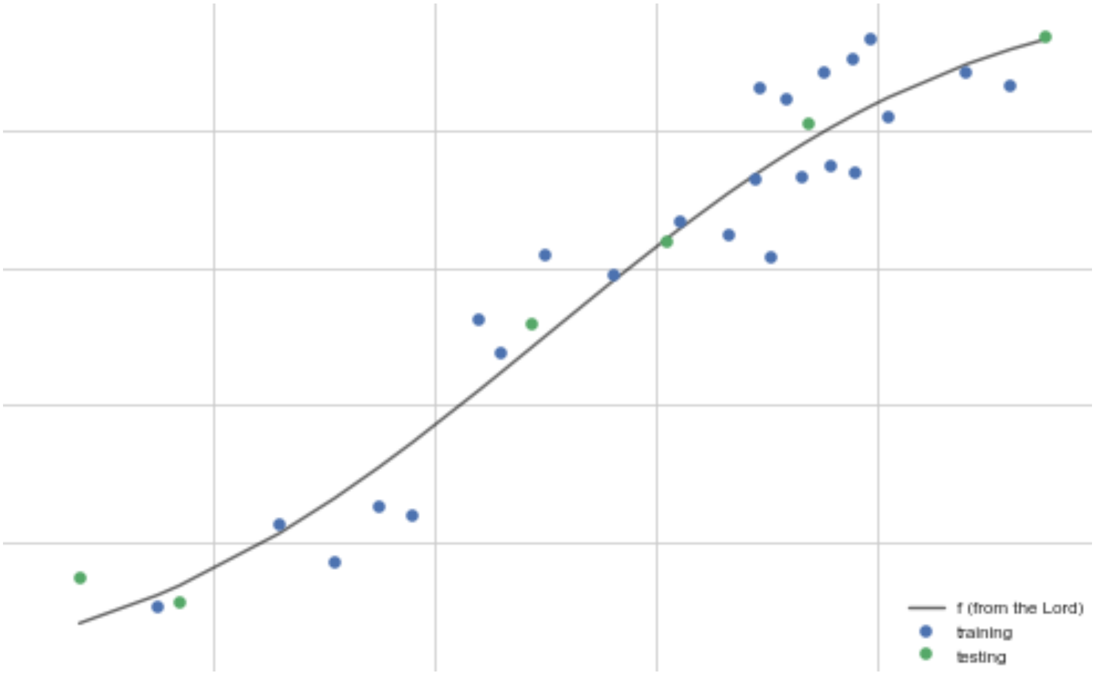
TRAIN AND TEST



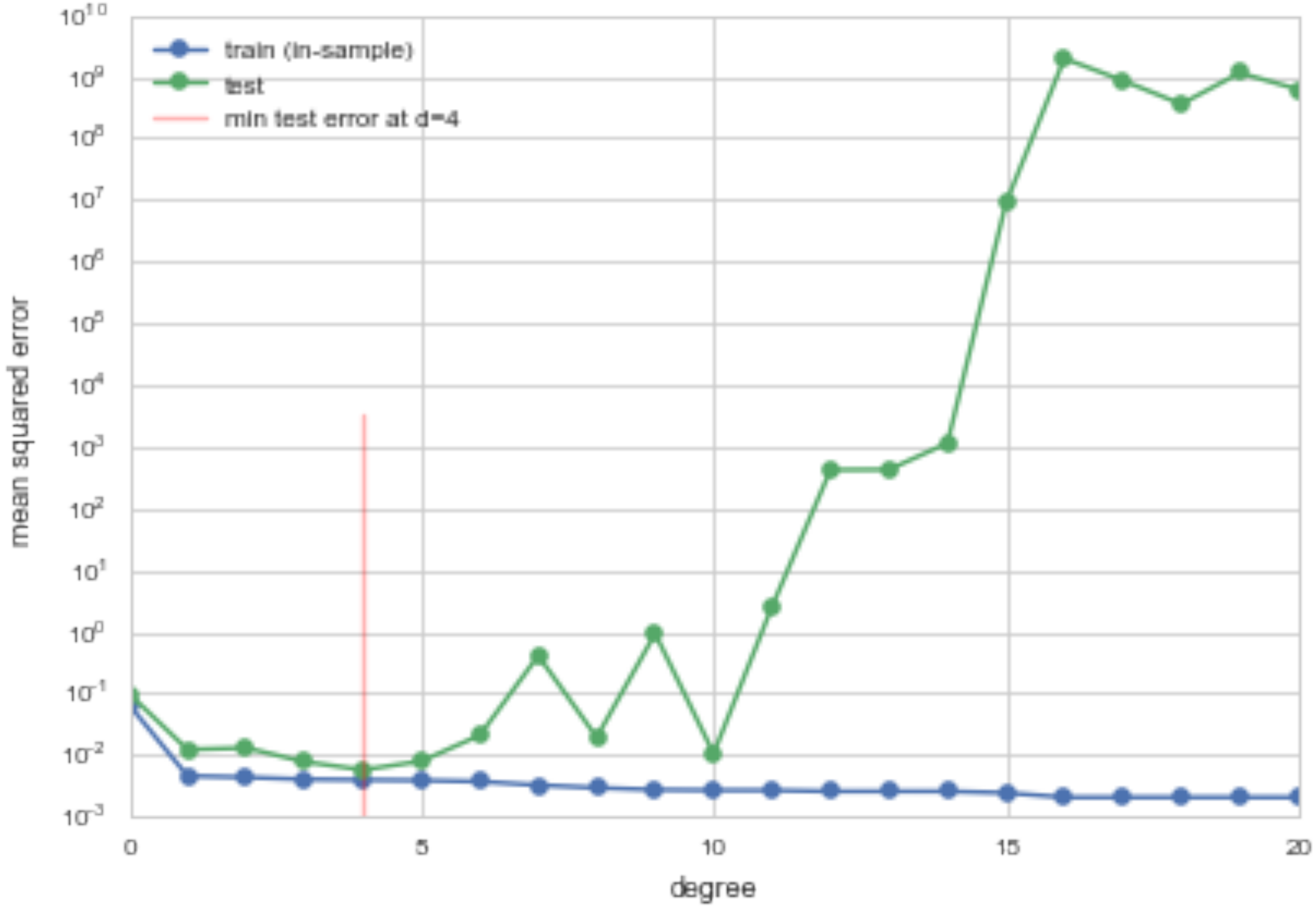


MODEL COMPARISON: A Large World approach





We "fit" for d



train (in-sample)
test
min test error at d=4
mean squared error
degree
10^{10}
10^{9}
10^{8}
10^{7}
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
0
5
10
15
20

Do we still have a test set?

Trouble:

- no discussion on the error bars on our error estimates
- "visually fitting" a value of $d \implies$ contaminated test set.

The moment we **use it in the learning process, it is not a test set**.

Hoeffding's inequality

population fraction μ, sample drawn with replacement, fraction ν:

$$P(|\nu - \mu| > \epsilon) \leq 2e^{-2\epsilon^2 N}$$

For hypothesis h, identify 1 with $h(x_i) \neq f(x_i)$ at sample x_i. Then μ, ν are population/sample error rates. Then,

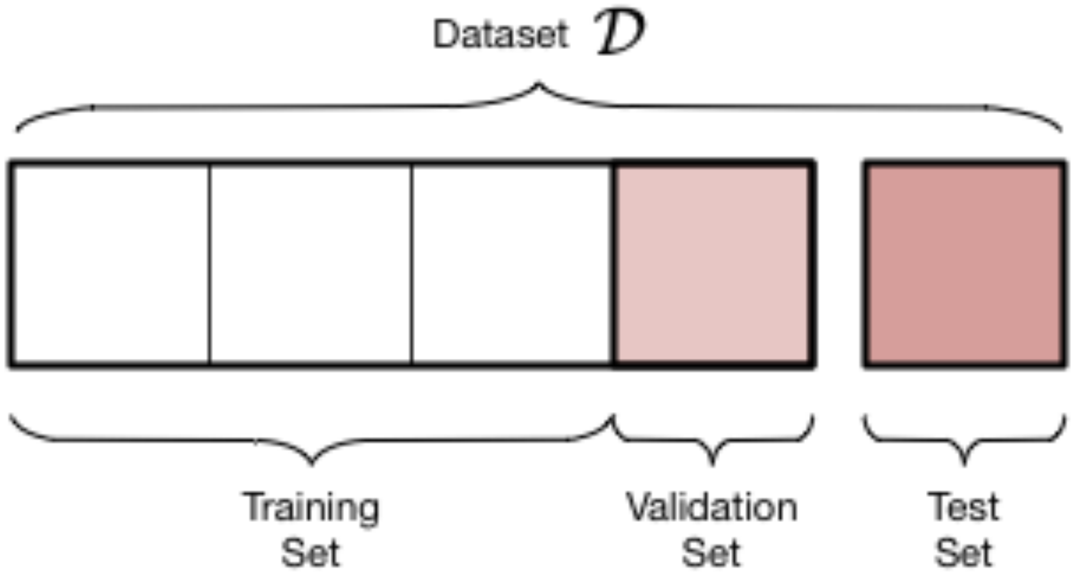
$$P(|R_{in}(h) - R_{out}(h)| > \epsilon) \leq 2e^{-2\epsilon^2 N}$$

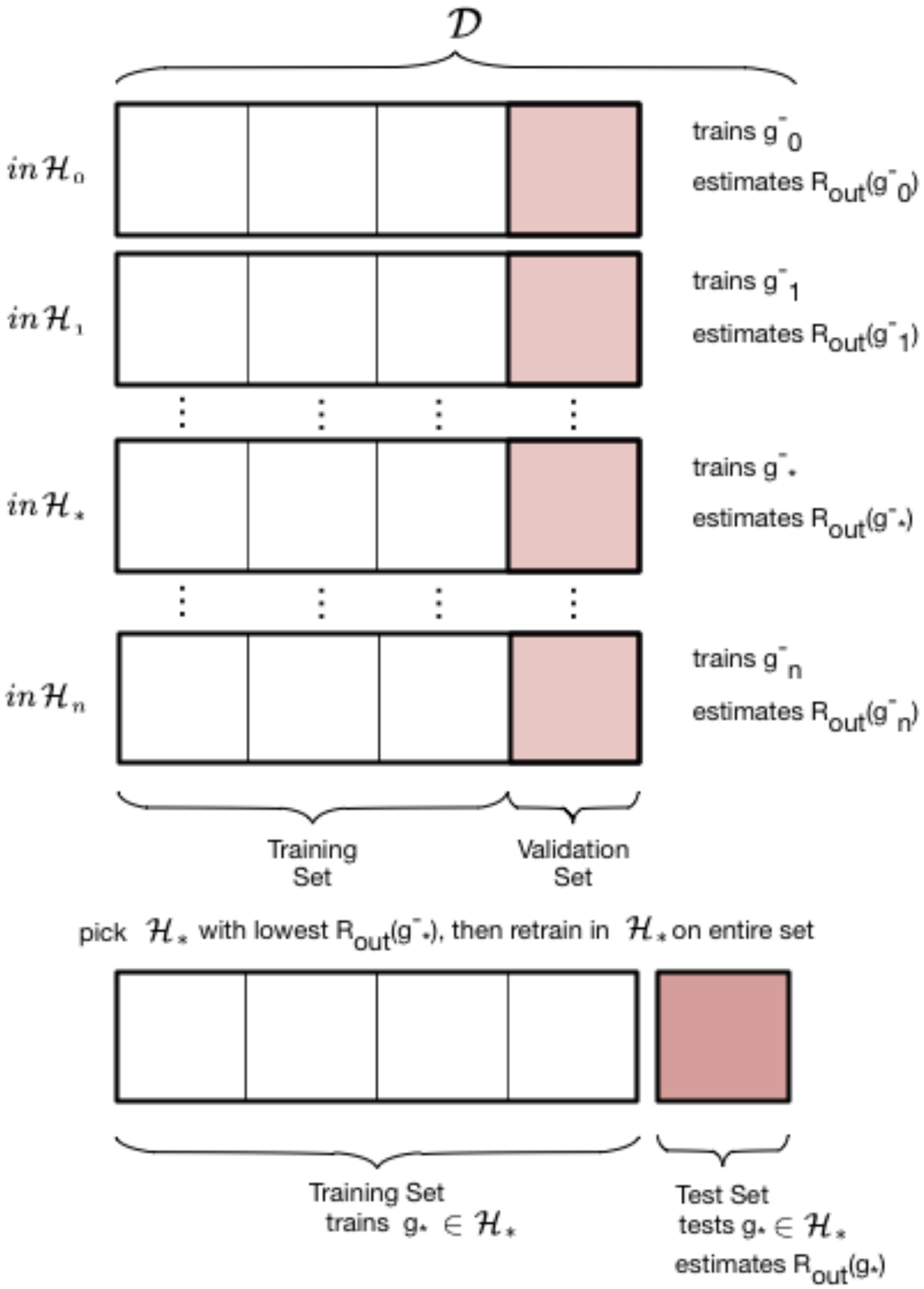
- Hoeffding inequality holds ONCE we have picked a hypothesis h, as we need it to label the 1 and 0s.
- But over the training set we one by one pick all the models in the hypothesis space
- best fit g is among the h in $\mathcal{H}$, g must be h_1 OR h_2 OR....Say **effectively** M such choices:

$$P(|R_{in}(g) - R_{out}(g)| \geq \epsilon) <= \sum_{h_i \in \mathcal{H}} P(|R_{in}(h_i) - R_{out}(h_i)| \geq \epsilon) <= 2\, M\, e^{-2\epsilon^2 N}$$

VALIDATION

- train-test not enough as we *fit* for d on test set and contaminate it
- thus do train-validate-test





pick $\mathcal{H}_*$ with lowest $R_{out}(g^-_*)$, then retrain in $\mathcal{H}_*$ on entire set

usually we want to fit a hyperparameter

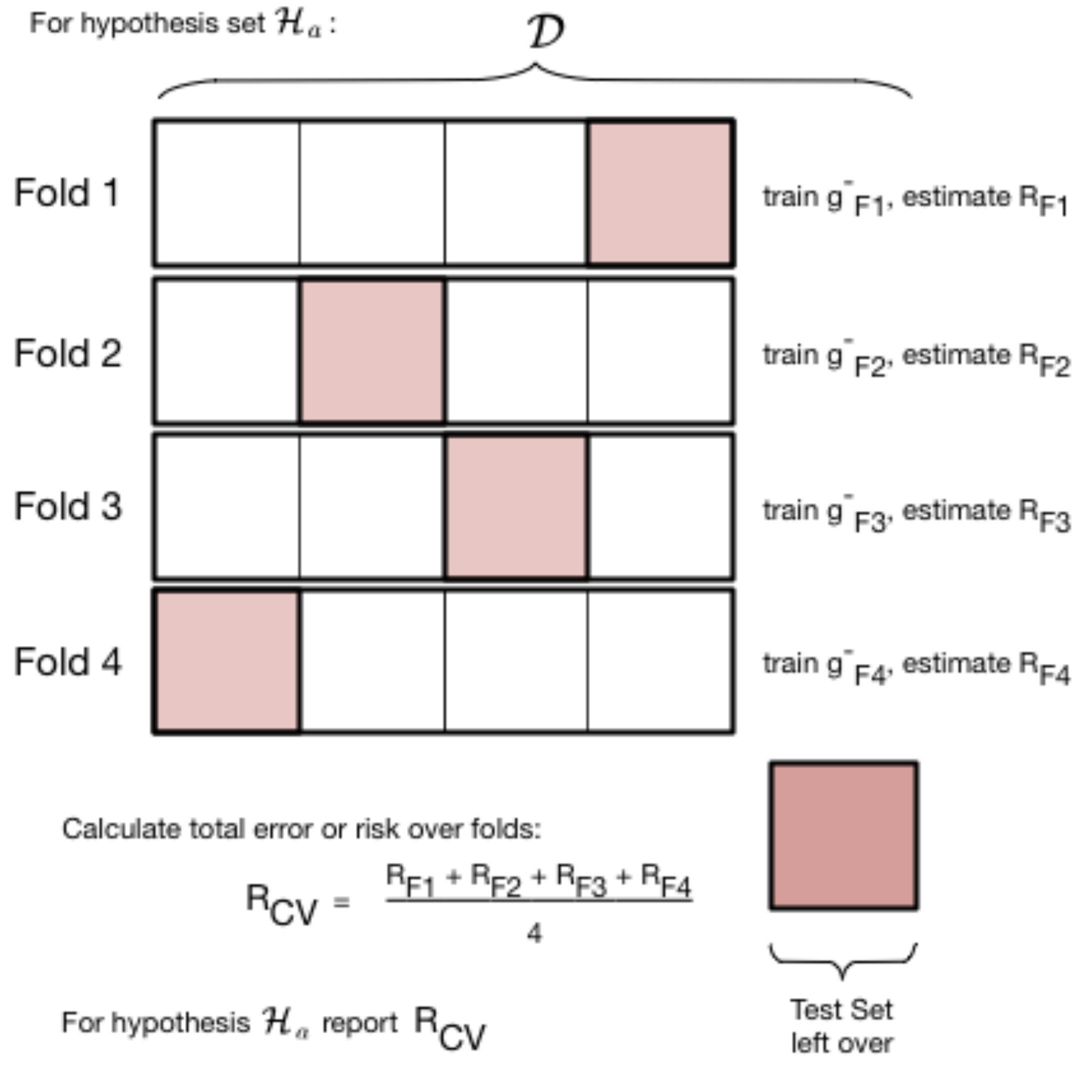
- we **wrongly** already attempted to fit d on our previous test set.
- choose the d, g^* combination with the lowest validation set risk.
- $R_{val}(g^{-*}, d^*)$ has an optimistic bias since d effectively fit on validation set
- its Hoeffding bound must now take into account the grid-size as the effective size of the hypothesis

- this size from hyperparameters is typically a smaller size than that from parameters.

Retrain on entire set!

- finally retrain on the entire train+validation set using the appropriate (g^{-*}, d^*) combination.
- works as training for a given hypothesis space with more data typically reduces the risk even further.
- test set has a M of 1!

CROSS-VALIDATION



For hypothesis set $\mathcal{H}_a$:

$\mathcal{D}$

Fold 1 train g^{-}_{F1}, estimate R_{F1}

Fold 2 train g^{-}_{F2}, estimate R_{F2}

Fold 3 train g^{-}_{F3}, estimate R_{F3}

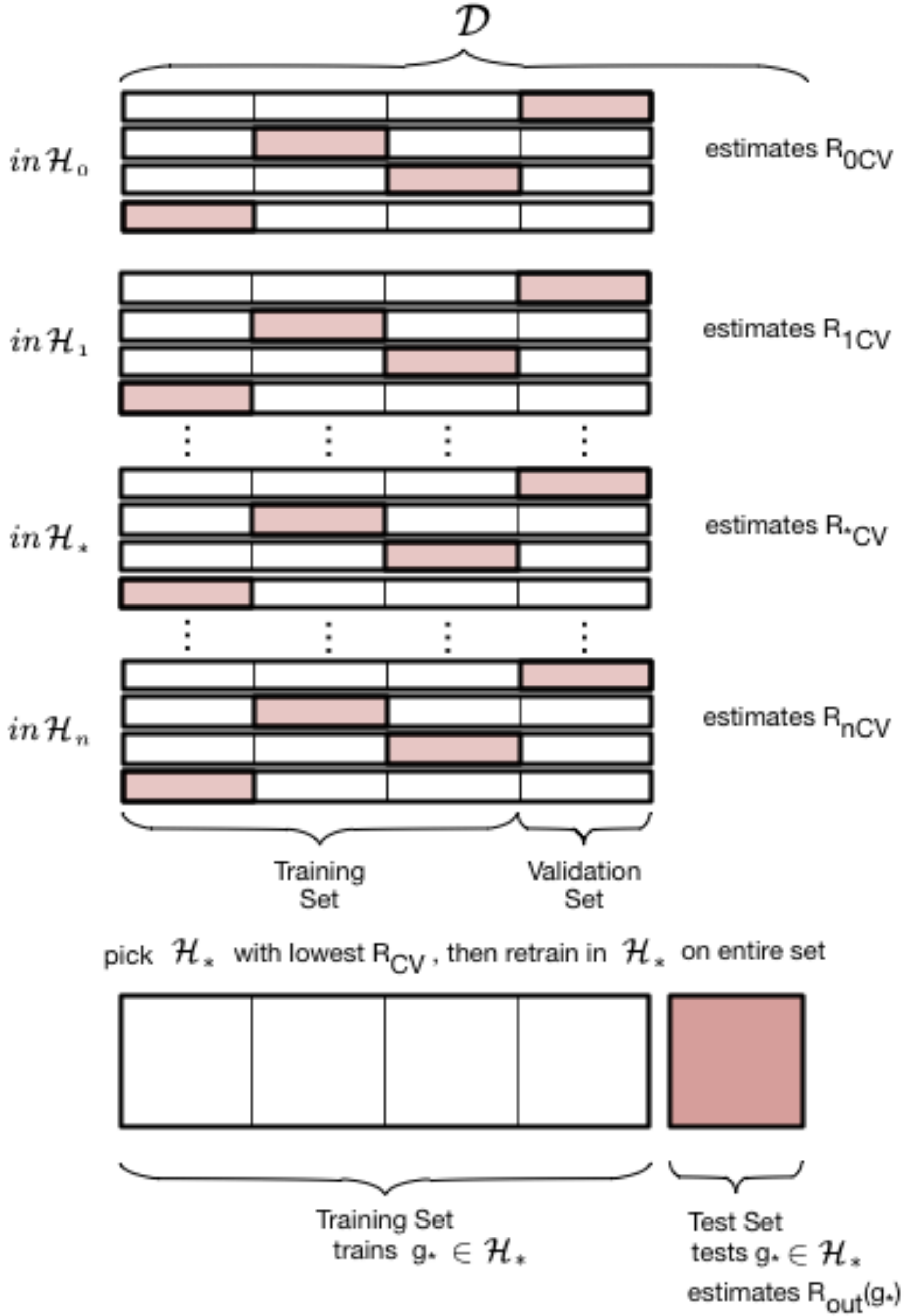
Fold 4 train g^{-}_{F4}, estimate R_{F4}

Calculate total error or risk over folds:

$$R_{CV} = \frac{R_{F1} + R_{F2} + R_{F3} + R_{F4}}{4}$$

For hypothesis $\mathcal{H}_a$ report R_{CV}

Test Set left over



$\mathcal{D}$

$in\, \mathcal{H}_0$ estimates R_{0CV}

$in\, \mathcal{H}_1$ estimates R_{1CV}

$in\, \mathcal{H}_*$ estimates R_{*CV}

$in\, \mathcal{H}_n$ estimates R_{nCV}

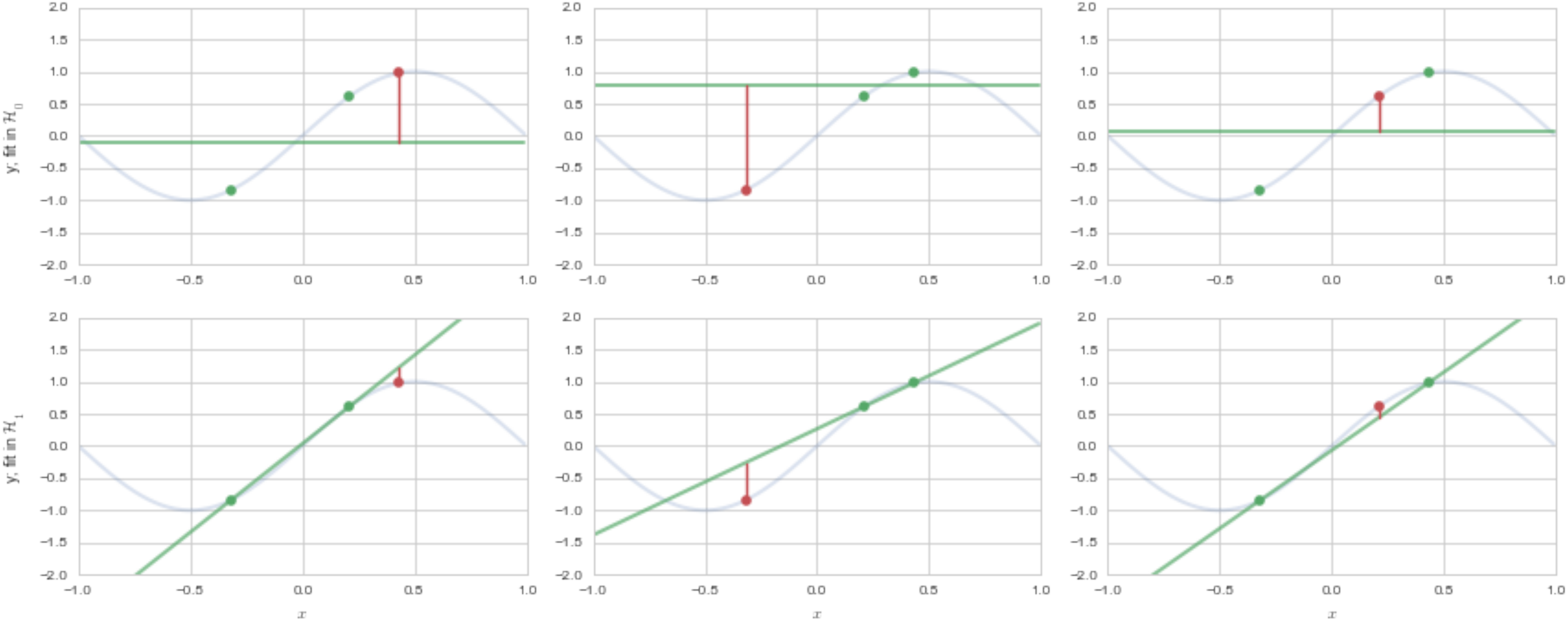
Training Set

Validation Set

pick $\mathcal{H}_*$ with lowest R_{CV}, then retrain in $\mathcal{H}_*$ on entire set

Training Set trains $g_* \in \mathcal{H}_*$

Test Set tests $g_* \in \mathcal{H}_*$ estimates $R_{out}(g_*)$

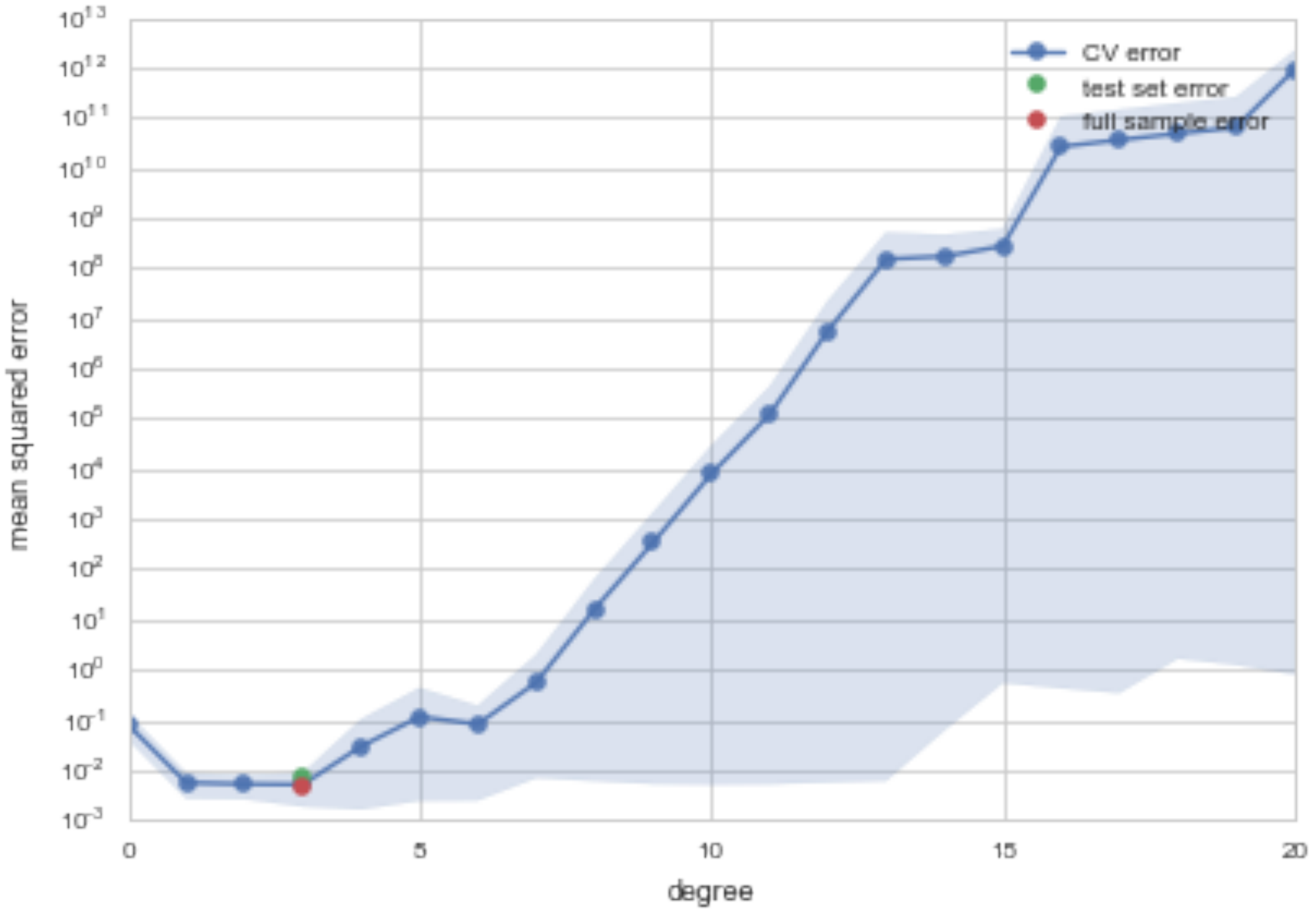

y; fit in $\mathcal{H}_0$
y; fit in $\mathcal{H}_1$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−1.0
−0.5
0.0
0.5
1.0
x
x
x

CROSS-VALIDATION

is

- a resampling method
- robust to outlier validation set
- allows for larger training sets
- allows for error estimates

Here we find $d = 3$.



Cross Validation considerations

- validation process as one that estimates R_{out} directly, on the validation set. It's critical use is in the model selection process.
- once you do that you can estimate R_{out} using the test set as usual, but now you have also got the benefit of a robust average and error bars.
- key subtlety: in the risk averaging process, you are actually averaging over different g^{-} models, with different parameters.

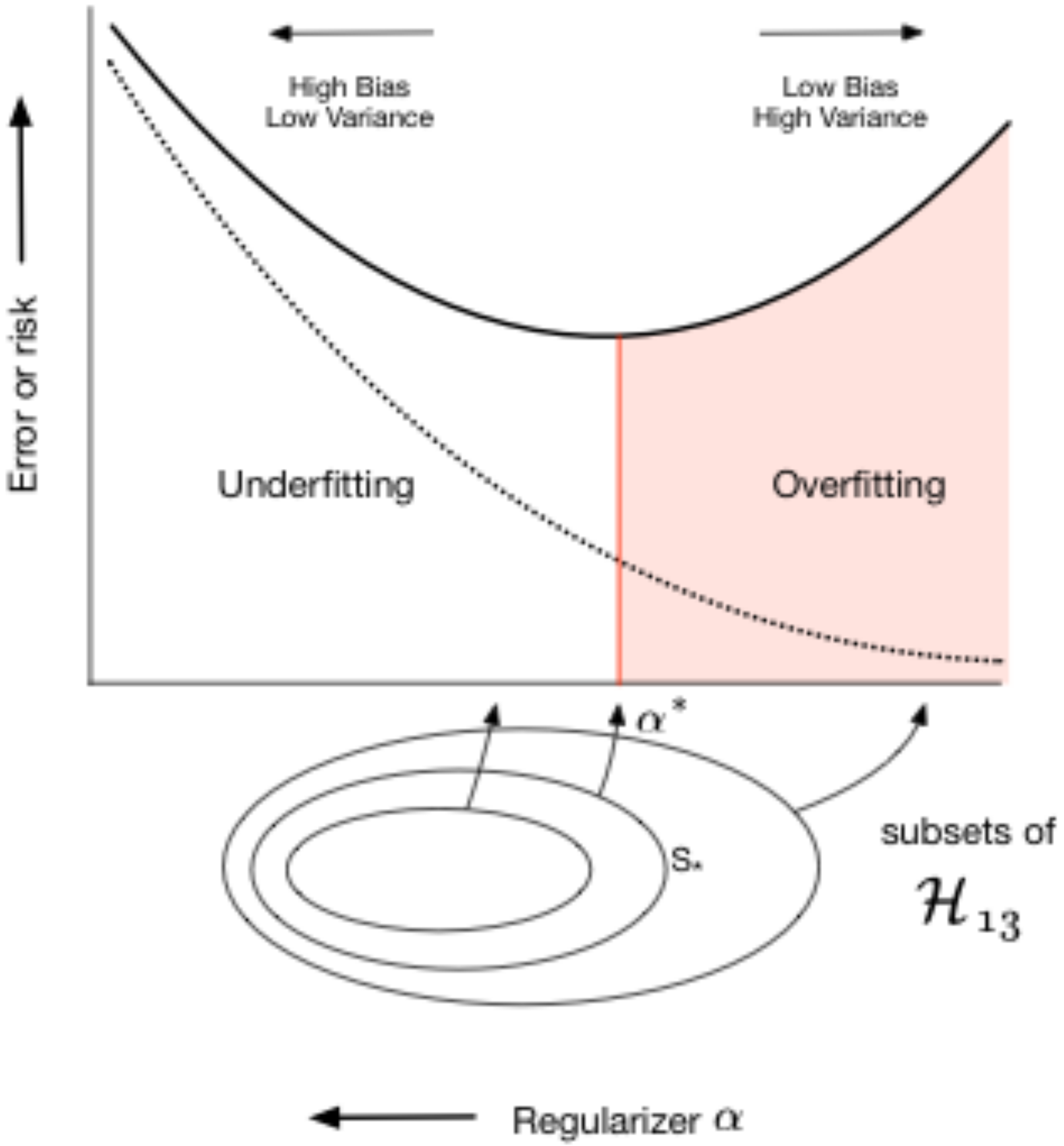
REGULARIZATION: A SMALL WORLD APPROACH

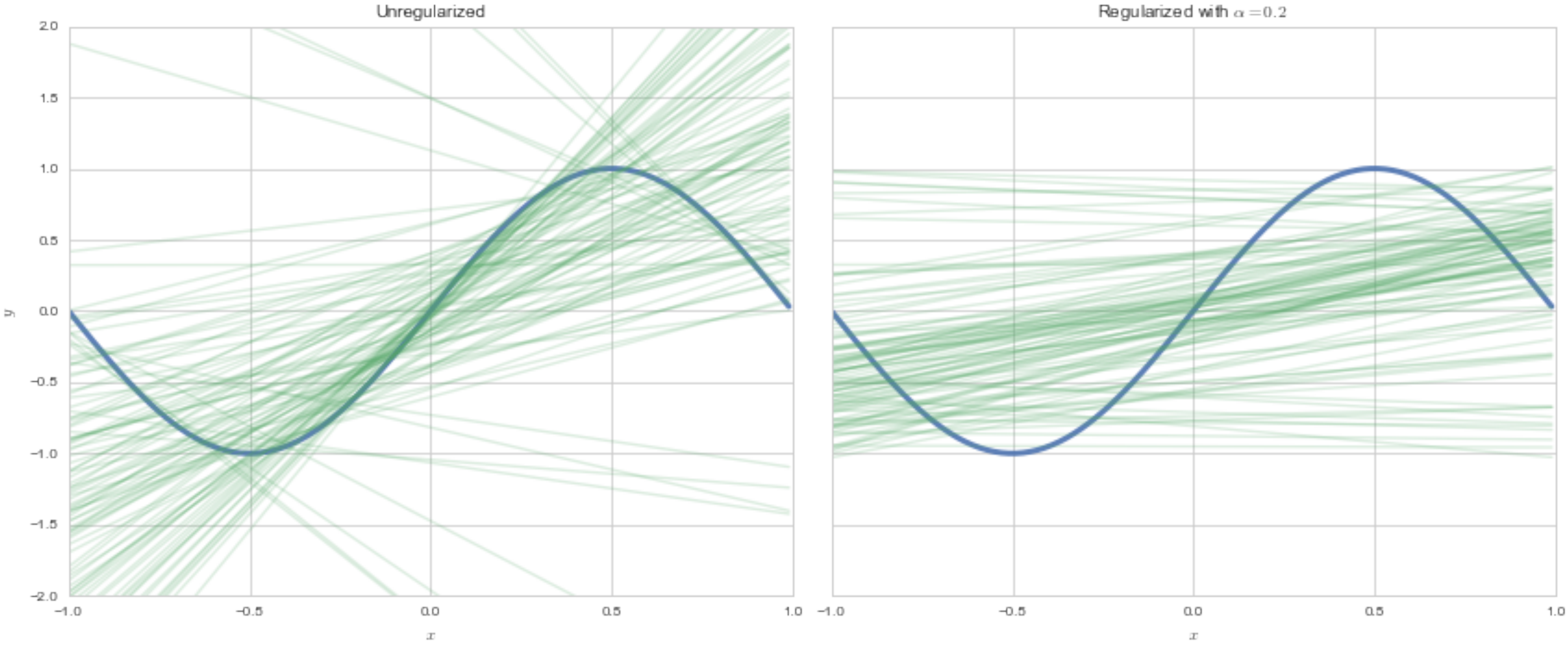
Keep higher a-priori complexity and impose a

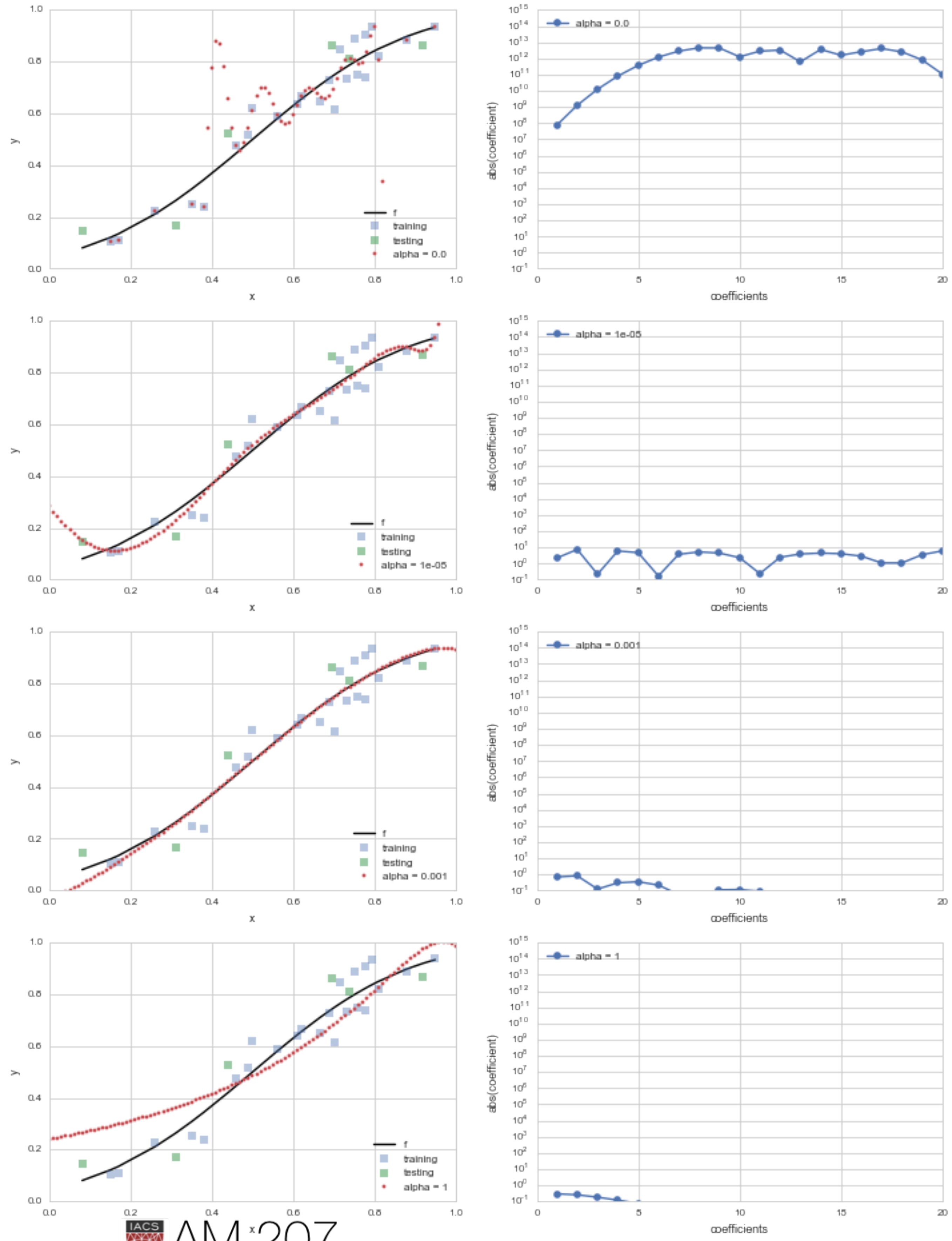
complexity penalty

on risk instead, to choose a SUBSET of $\mathcal{H}_{big}$. We'll make the coefficients small:

$$\sum_{i=0}^{j} \theta_i^2 < C.$$




Unregularized
Regularized with $\alpha = 0.2$
y
x
x
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−1.0
−0.5
0.0
0.5
1.0



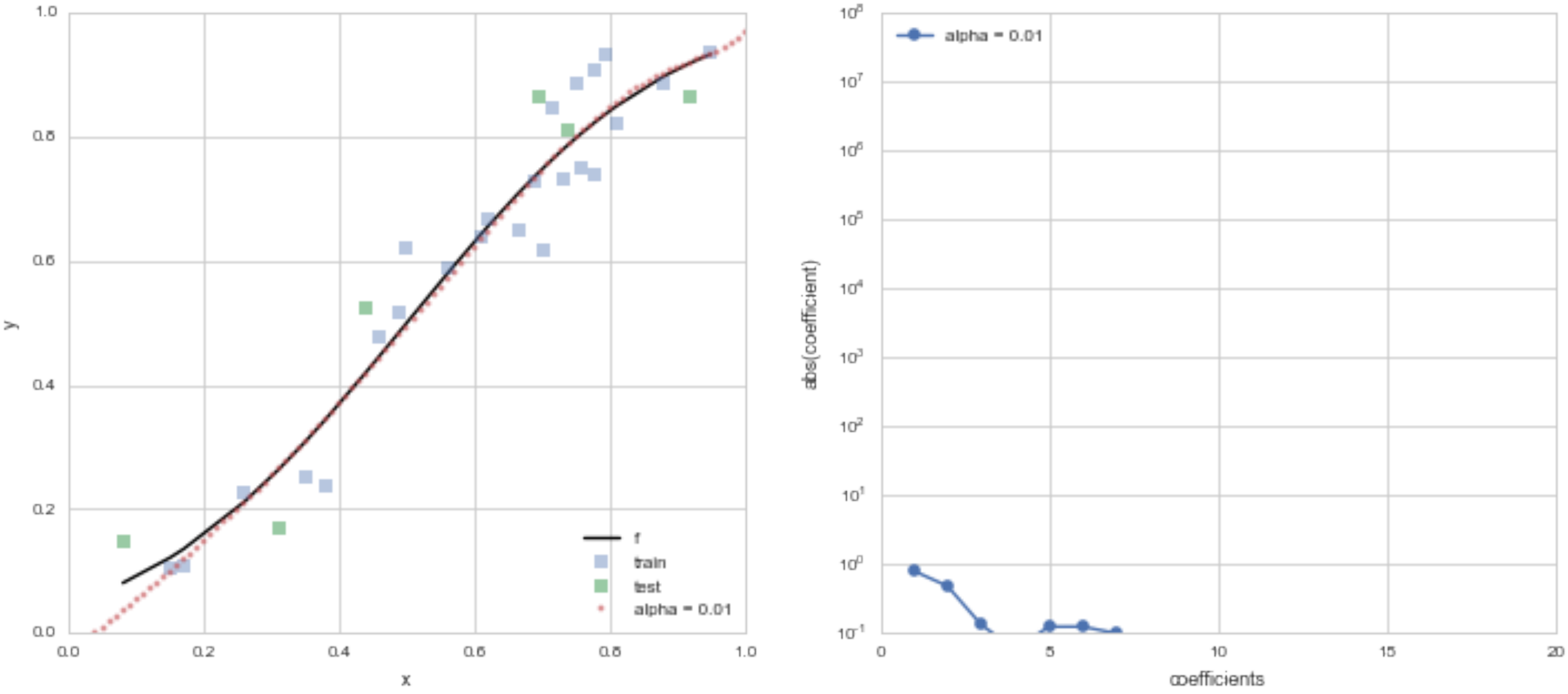
REGULARIZATION

$$\mathcal{R}(h_j) = \sum_{y_i \in \mathcal{D}} (y_i - h_j(x_i))^2 + \alpha \sum_{i=0}^{j} \theta_i^2 .$$

As we increase α, coefficients go towards 0.

Lasso uses $\alpha \sum_{i=0}^{j} |\theta_i|$, sets coefficients to exactly 0.

Regularization with Cross-Validation



MODEL COMPARISON: In-sample estimation

- Suppose we have a large-world subset of nested models.
- .. thus the models have the same likelihood form
- would be nice to not have to spend data on validation sets
- and exploit the notion that a negative log likelihood is a loss
- we could use strength of effects
- but not really needed for prediction

KL-Divergence

$$D_{KL}(p,q) = E_p[log(p) - log(q)] = E_p[log(p/q)]$$
$$= \sum_i p_i log(\frac{p_i}{q_i}) \; or \int dPlog(\frac{p}{q})$$

$$D_{KL}(p,p) = 0$$

KL divergence measures distance/dissimilarity of the two distributions $p(x)$ and $q(x)$.

Divergence:

The additional uncertainty indiced by using probabilities from one distribution to describe another distribution

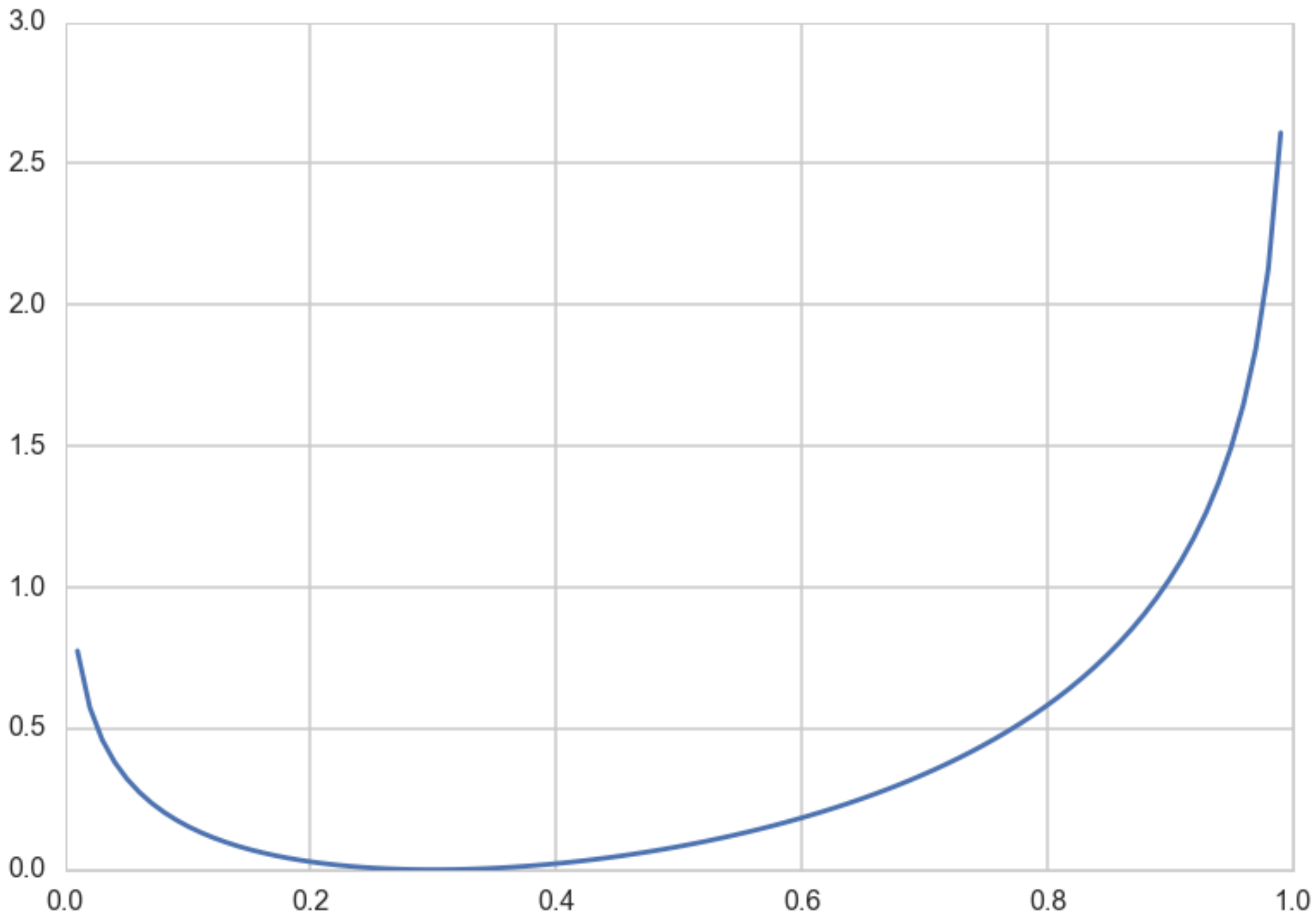
- McElreath page 179

KL example

Bernoulli Distribution p with $p = 0.3$.

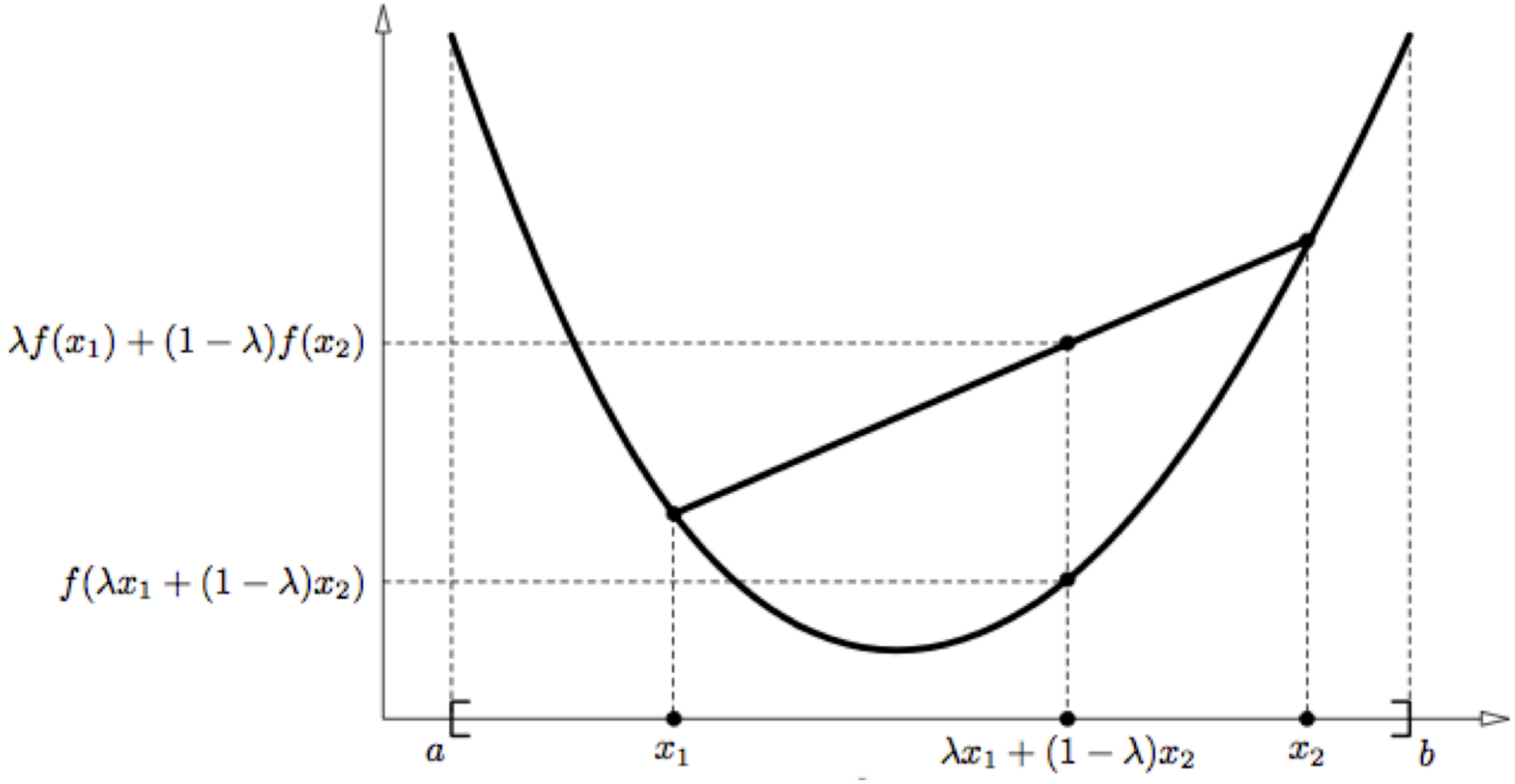
Try to approximate by q. What parameter?

```
def kld(p,q):
    return p*np.log(p/q) + (1-p)*np.log((1-p)/(1-q))
```



Jensen's Inequality for convex $f(x)$:

$$E[f(X)] \geq f(E[X])$$



$\lambda f(x_1) + (1-\lambda) f(x_2)$
$f(\lambda x_1 + (1-\lambda) x_2)$
a
x_1
$\lambda x_1 + (1-\lambda) x_2$
x_2
b

KL-Divergence is always non-negative

Jensen's inequality:

$\implies D_{KL}(p,q) \geq 0$ (0 iff $q = p \, \forall x$).

$$D_{KL}(p,q) = E_p[log(p/q)] = E_p[-log(q/p)] \geq -\log(E_p[q/p]) = -\log(\int dQ) = 0$$

MARS ATTACKS (Topps, 1962; Burton 1996)

$$Earth : q = \{0.7, 0.3\}, Mars : p = \{0.01, 0.99\}.$$

Earth to predict Mars, less surprise on landing: $D_{KL}(p, q) = 1.14, D_{KL}(q, p) = 2.62$.

PROBLEM: we dont know distribution p. If we did, why do inference?

SOLUTION: Use the empirical distribution

That is, approximate population expectations by sample averages.

$$\implies D_{KL}(p,q) = E_p[log(p/q)] = \frac{1}{N}\sum_i log(p_i/q_i)$$

Maximum Likelihood justification

$$D_{KL}(p,q) = E_p[log(p/q)] = \frac{1}{N}\sum_i (log(p_i) - log(q_i))$$

Minimizing KL-divergence $\implies$ maximizing $\sum_i log(q_i)$

Which is exactly the log likelihood! MLE!

Model Comparison: Likelihood Ratio

$$D_{KL}(p,q) - D_{KL}(p,r) = E_p[log(r) - log(q)] = E_p[log(\frac{r}{q})]$$

In the sample approximation we have:

$$D_{KL}(p,q) - D_{KL}(p,r) = \frac{1}{N}\sum_i log(\frac{r_i}{q_i}) = \frac{1}{N} log(\frac{\prod_i r_i}{\prod_i q_i}) = \frac{1}{N} log(\frac{\mathcal{L}_r}{\mathcal{L}_q})$$

MODEL COMPARISON: Deviance

You only need the sample averages of the logarithm of r and q:

$$D_{KL}(p,q) - D_{KL}(p,r) = \langle log(r) \rangle - \langle log(q) \rangle$$

Define the deviance: $D(q) = -2 \sum_i log(q_i)$, a **LOSS** ...

$$D_{KL}(p,q) - D_{KL}(p,r) = \frac{2}{N}(D(q) - D(r))$$

Example

Generate data from:

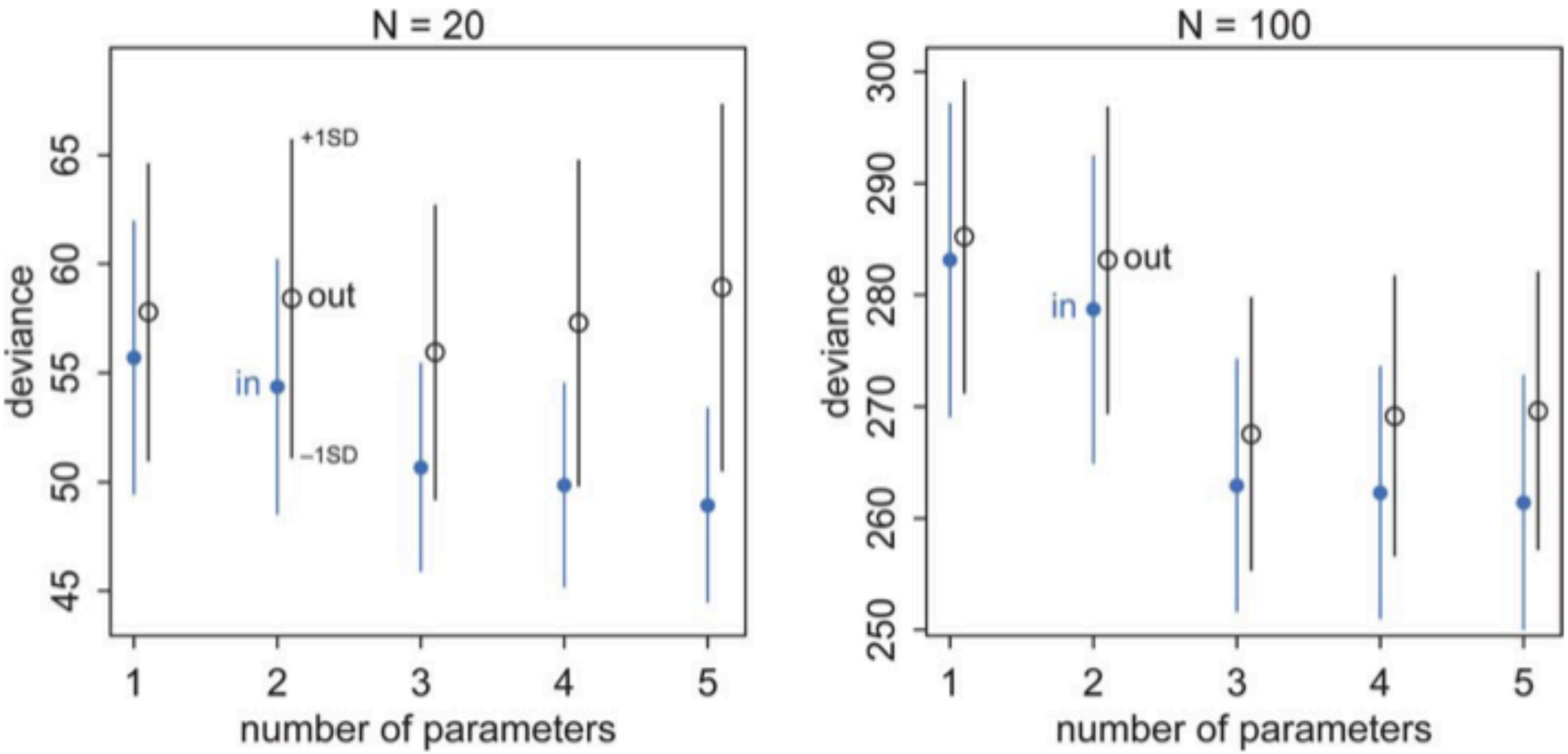
$$\mu_i = 0.15 x_{1,i} - 0.4 x_{2,i}\,,\;\; y \sim N(\mu, 1)$$

2 parameter model.

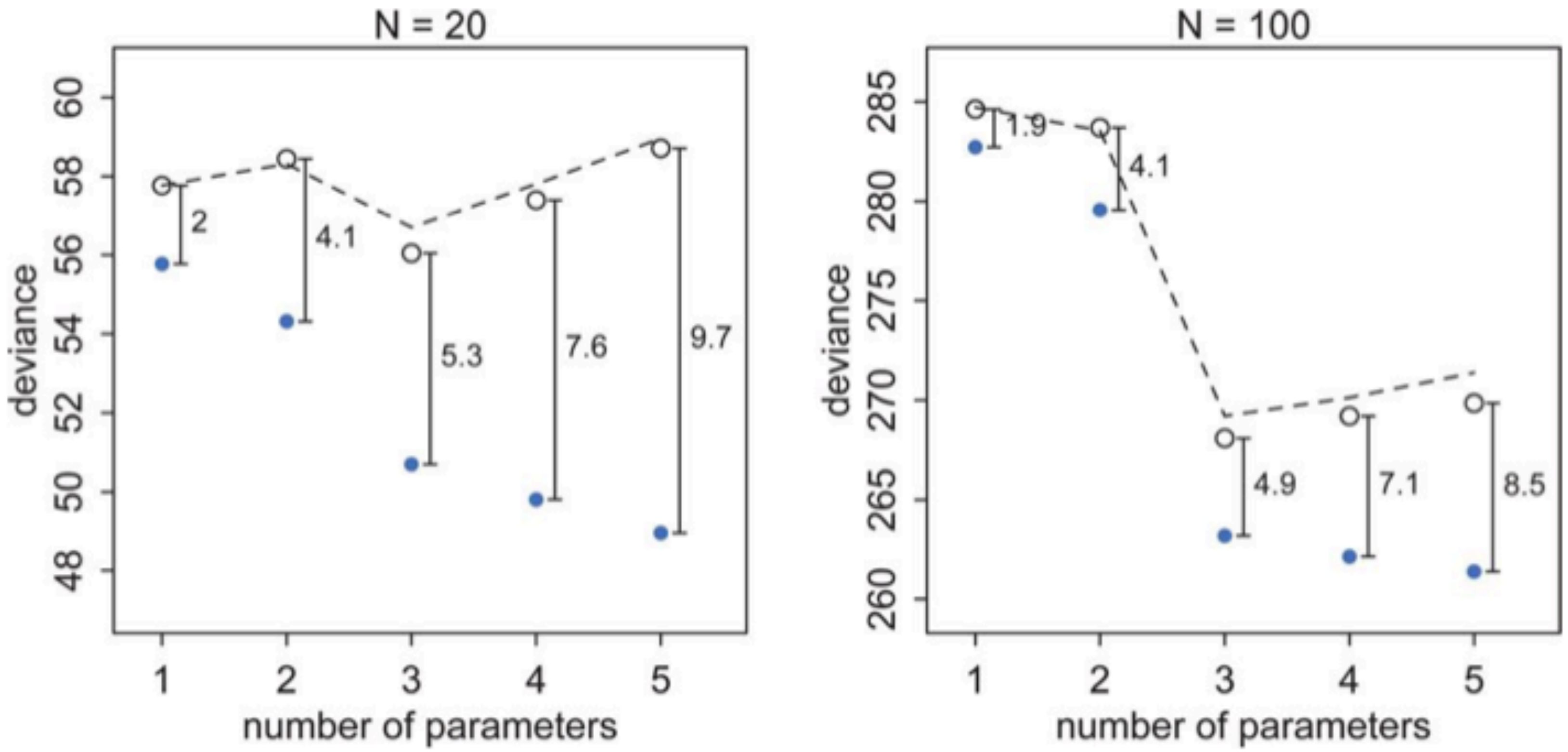
Generate 10,000 realizations, for 1-5 parameters, 20 data points and 100 data points.

Split into train and test, and do OLS.

Train and Test Deviances



Train and Test Deviances



The test set deviances are $2 * p$ above the training set ones.

Akake **Information Criterion**:

AIC **estimates out-of-sample deviance**

$$AIC = D_{train} + 2p$$

- Assumption: likelihood is approximately multivariate gaussian.
- penalized log-likelihood or risk if we choose to identify our distribution with the likelihood: REGULARIZATION

AIC for Linear Regression

$$AIC = D_{train} + 2p \text{ where}$$

$$D(q) = -2\sum_i log(q_i) = -2\ell$$

$$\sigma^2_{MLE} = \frac{1}{N} SSE$$

$$AIC = -2(-\frac{N}{2}(log(2\pi) + log(\sigma^2)) - 2(-\frac{1}{2\sigma^2_{MLE}} \times SSE) + 2p$$

$$AIC = Nlog(SSE/N) + 2p + constant$$