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

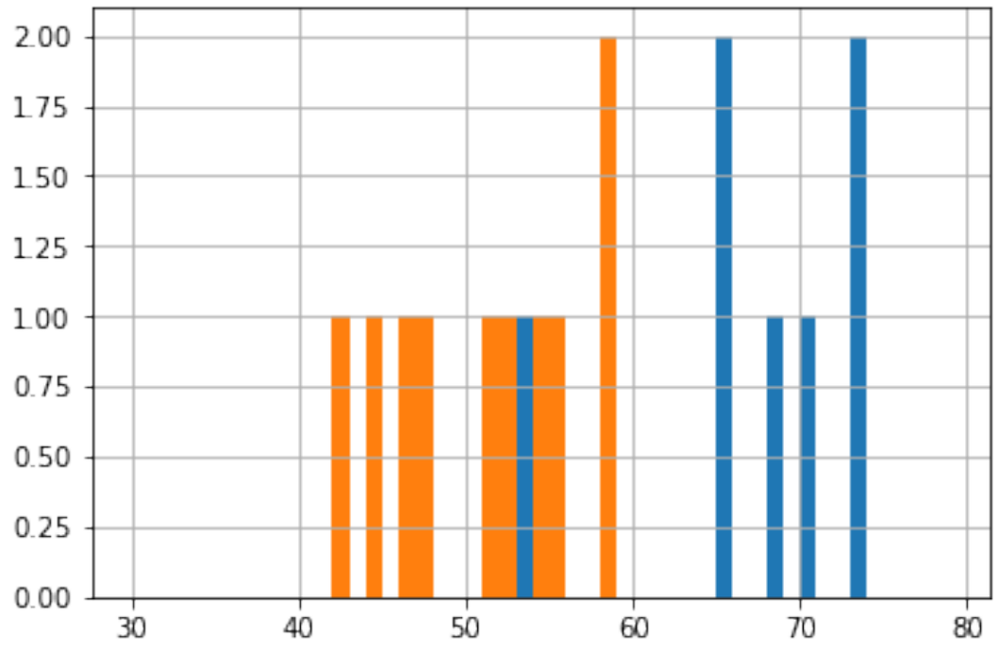
# Today

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

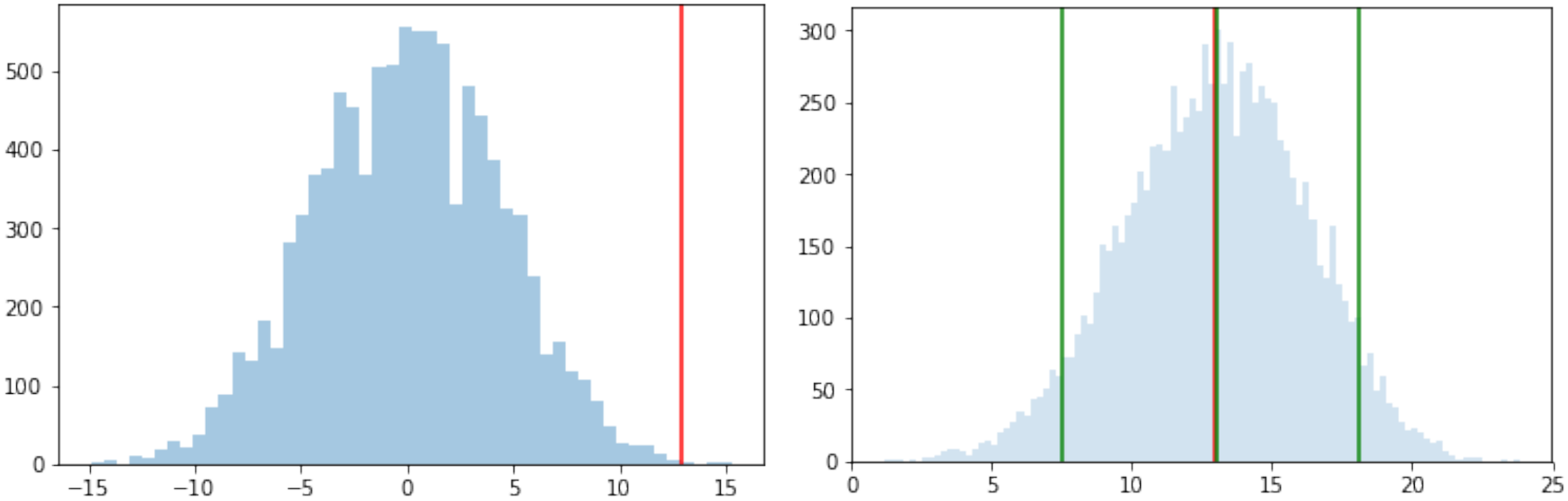
| | dosage | label |
|---|---|---|
| **0** | 54 | P |
| **1** | 51 | P |
| **2** | 58 | P |
| **3** | 44 | P |
| **4** | 55 | P |
| **5** | 52 | P |
| **6** | 42 | P |
| **7** | 47 | P |
| **8** | 58 | P |
| **9** | 46 | P |
| **10** | 54 | D |
| **11** | 73 | D |
| **12** | 53 | D |
| **13** | 70 |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

# Dose vs Placebo

Actual mean effect is about 13.



# Significance vs Size of Effect




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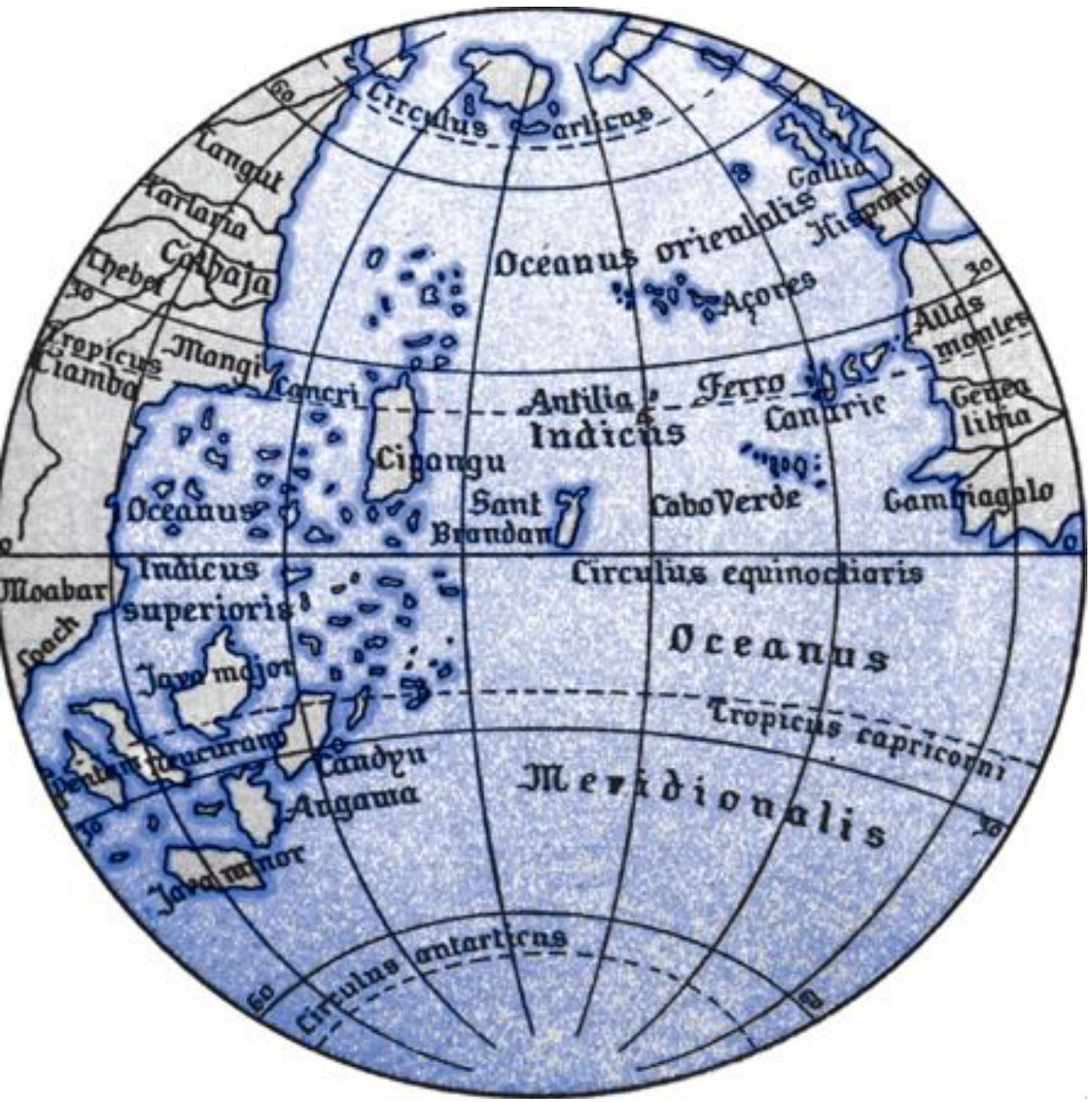
# HYPOTHESIS SPACES

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.

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

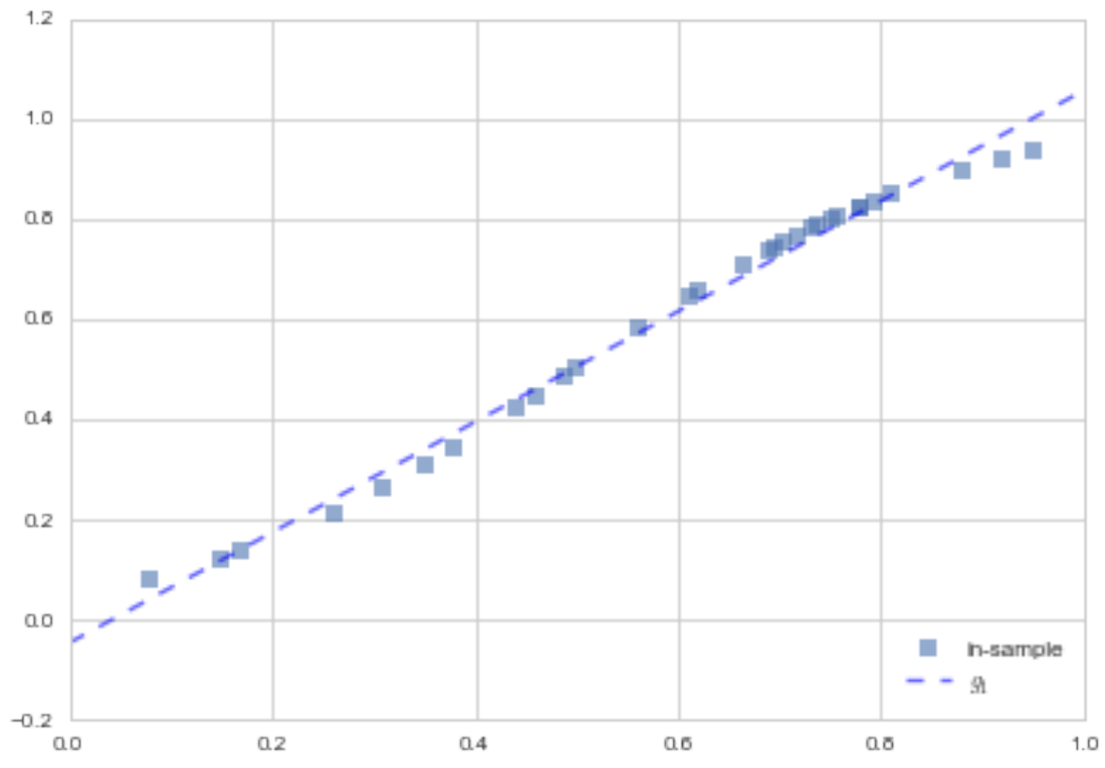


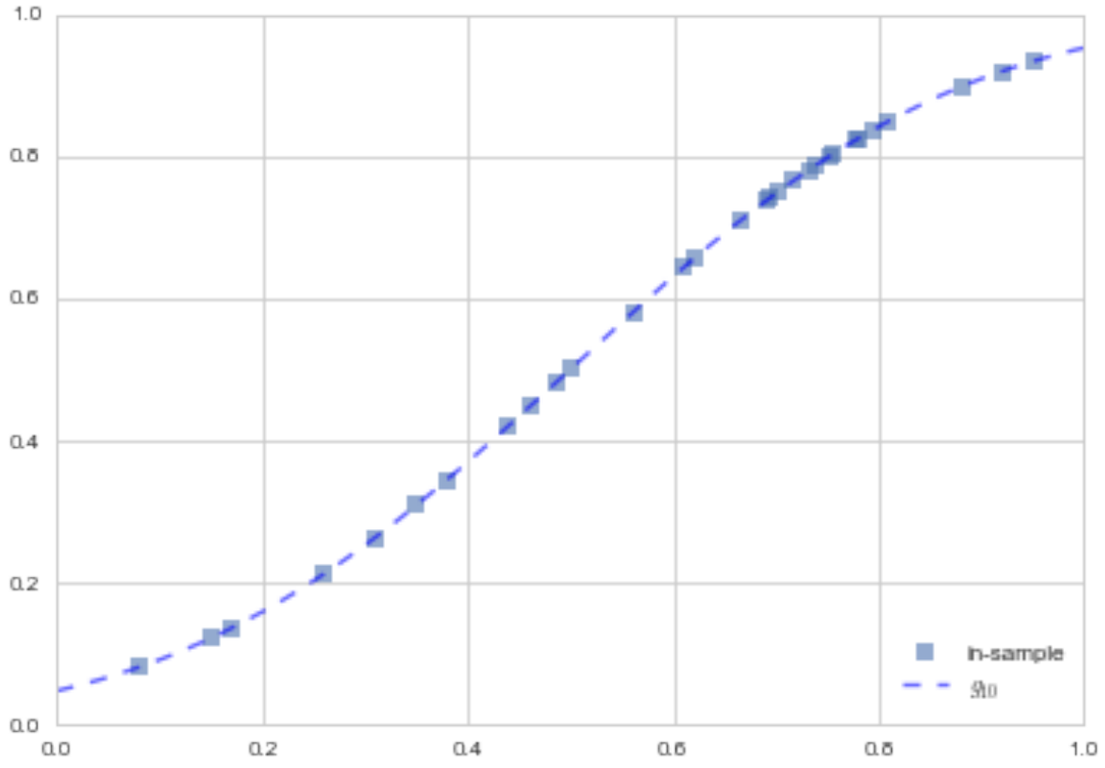

# SMALL World vs BIG World

- *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 $\mathcal{H}_{20}$?

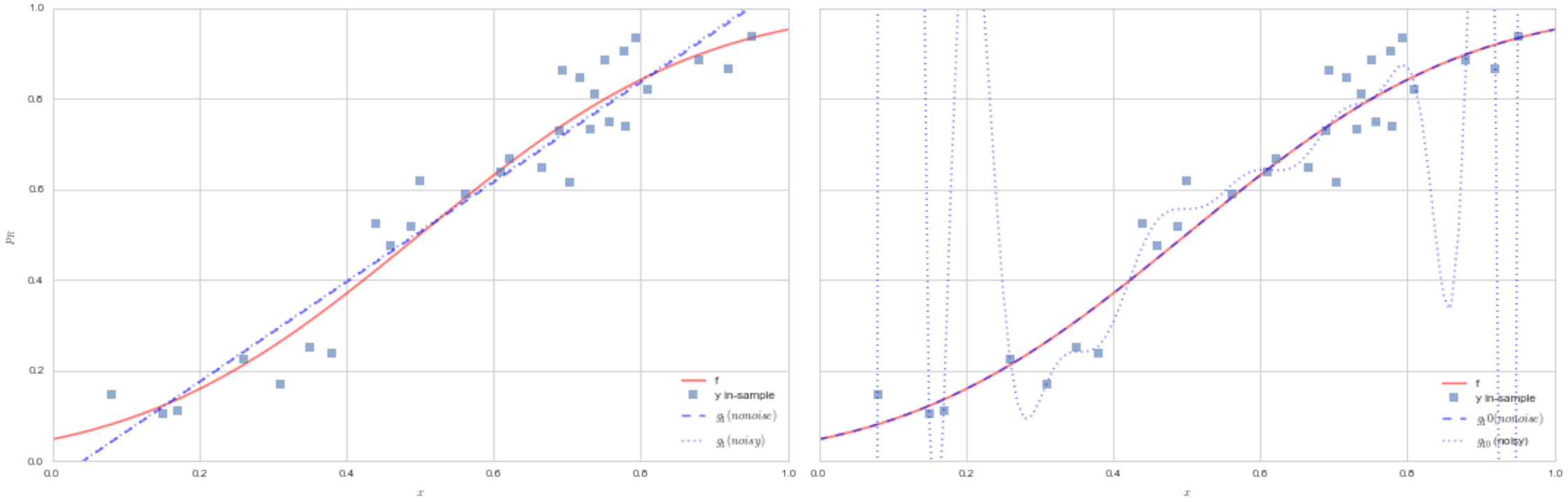


# THE REAL WORLD HAS NOISE

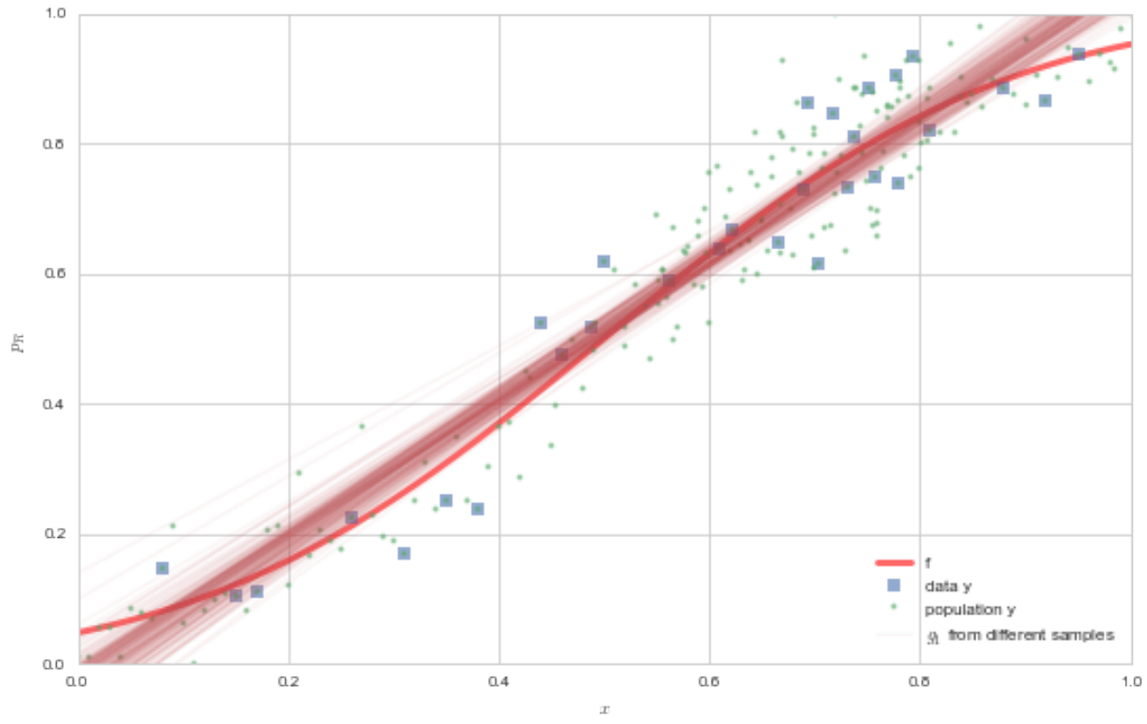
Which fit is better now?

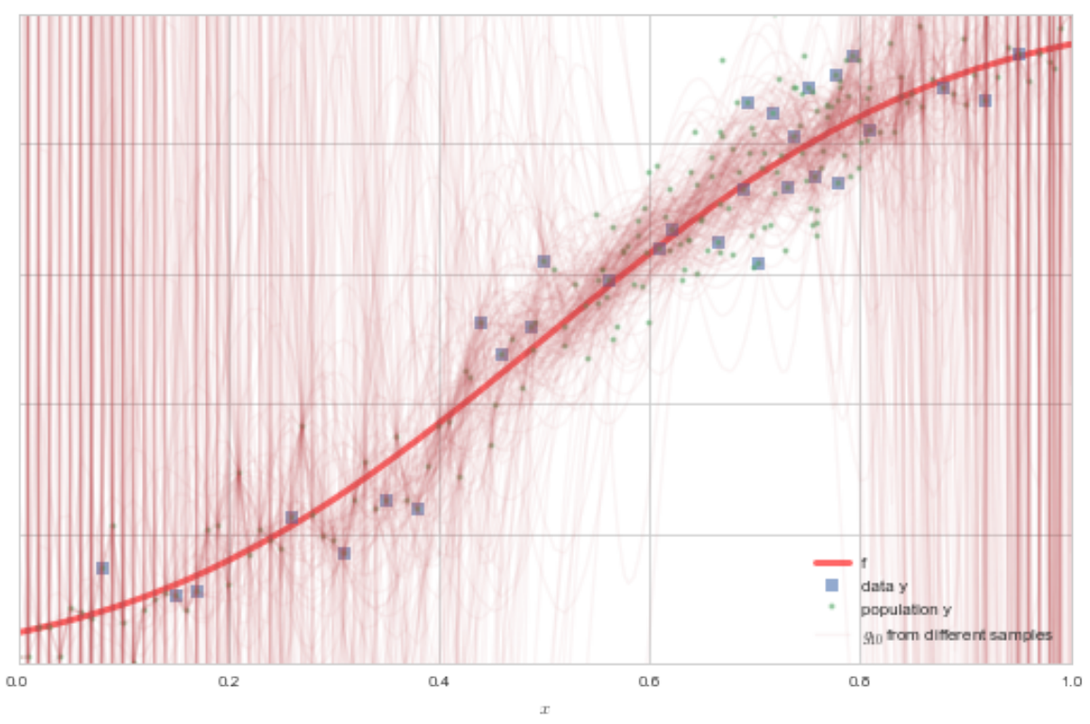
The line or the curve?



# UNDERFITTING (Bias)

# vs OVERFITTING (Variance)



# Every model has Bias and Variance

One sample, stochastic based on the sample you have

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

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

Define:

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

avg over M different samples, h(x) changes from one set of sample to the next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Ep - Expectation over x's
Ed - Expectation over dataset

gD is the fit over all possible dataset?

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

Avg of all possible fits

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

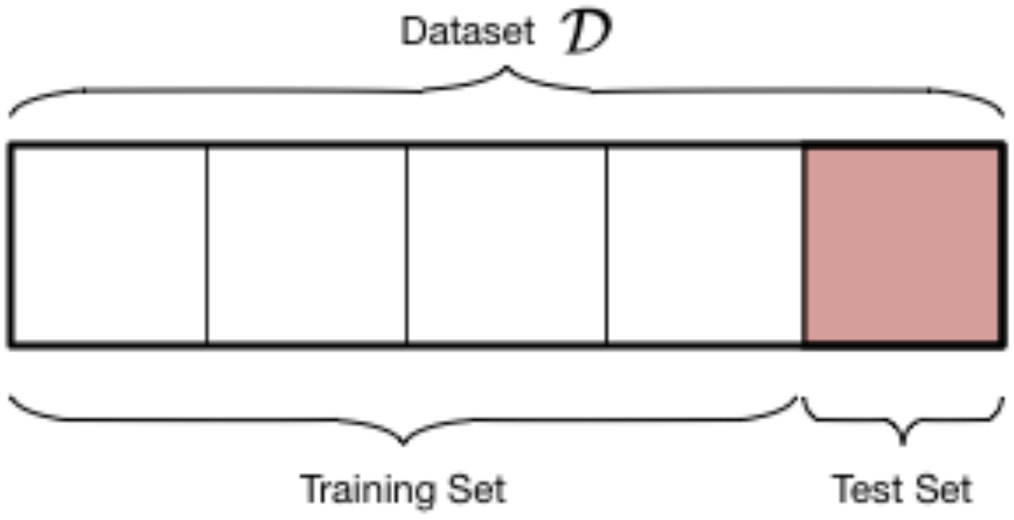
Then,

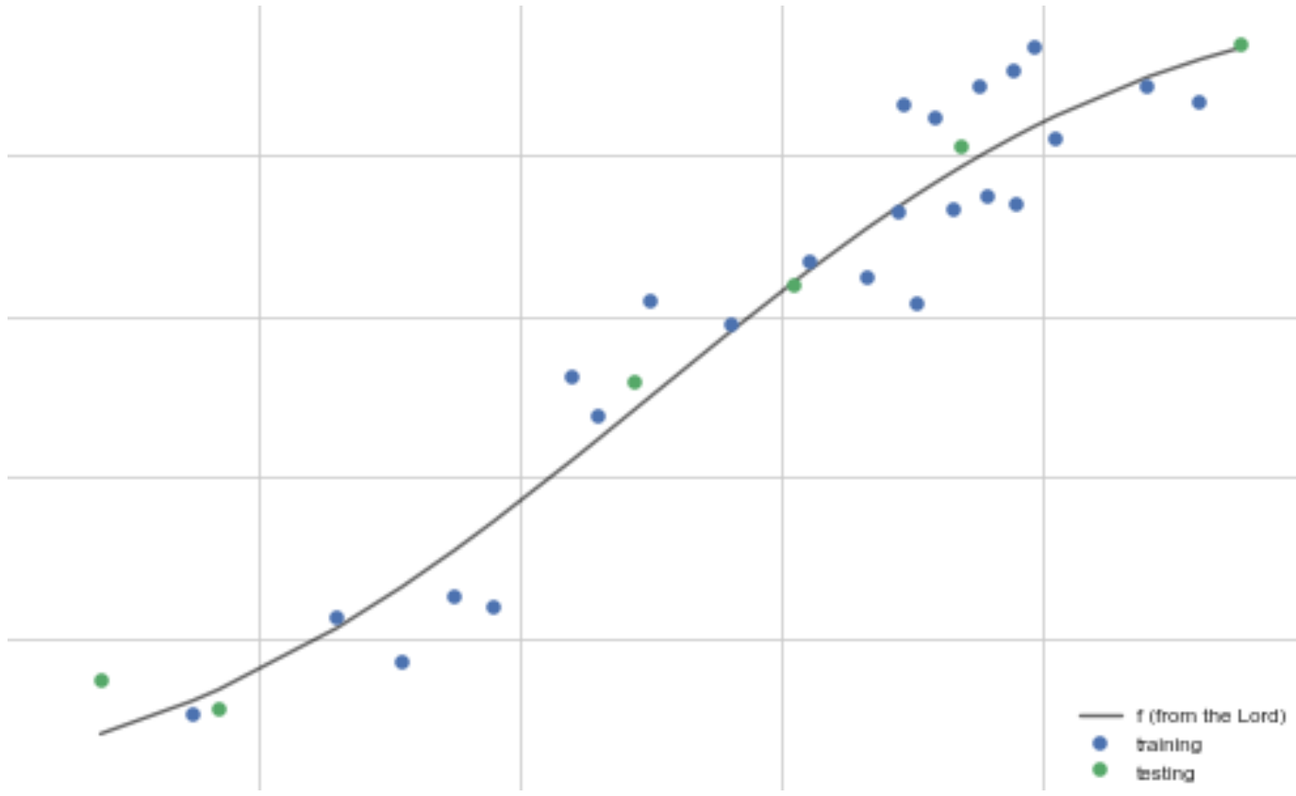
$$\langle R \rangle = E_{p(x)}[E_{\mathcal{D}}[(g_{\mathcal{D}} - \bar{g})^2]] + E_{p(x)}[(f - \bar{g})^2] + \sigma^2$$

This is the bias variance decomposition for regression.

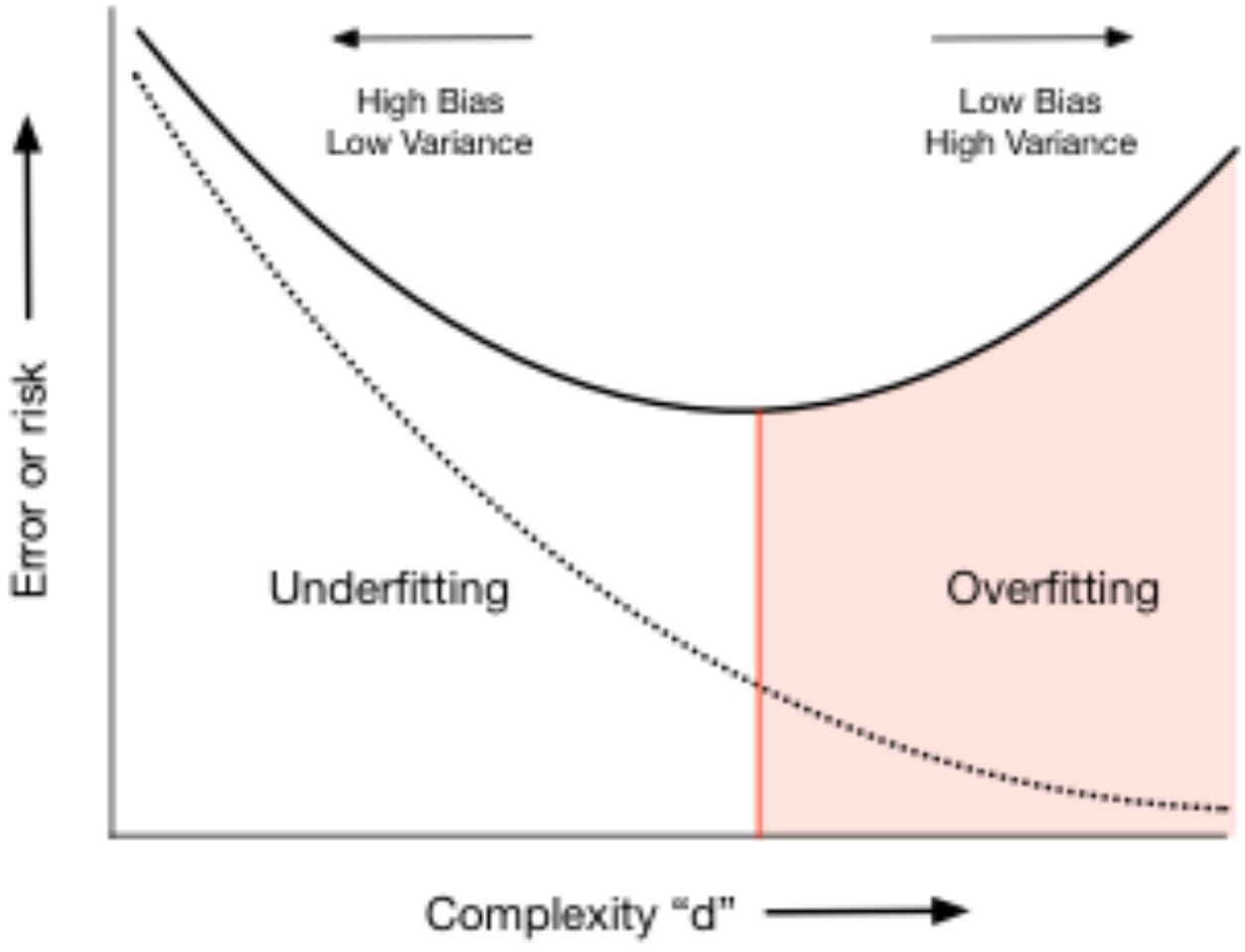
- first term is **variance**, squared error of the various fit g's from the average g, the hairiness.
- second term is **bias**, how far the average g is from the original f this data came from.
- third term is the **stochastic noise**, minimum error that this model will always have.

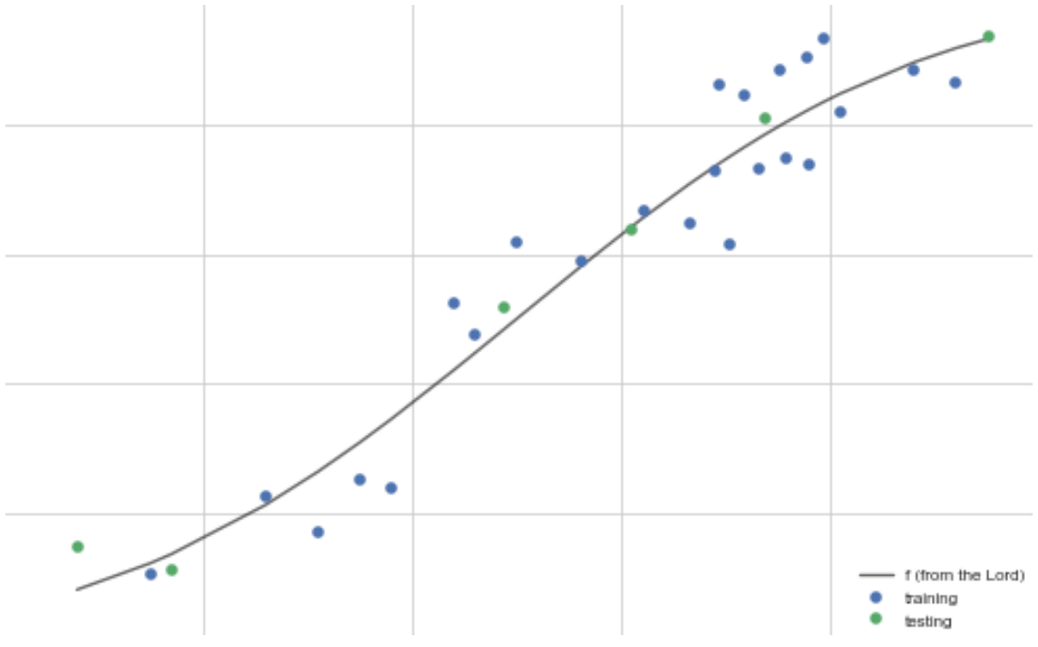
# TRAIN AND TEST



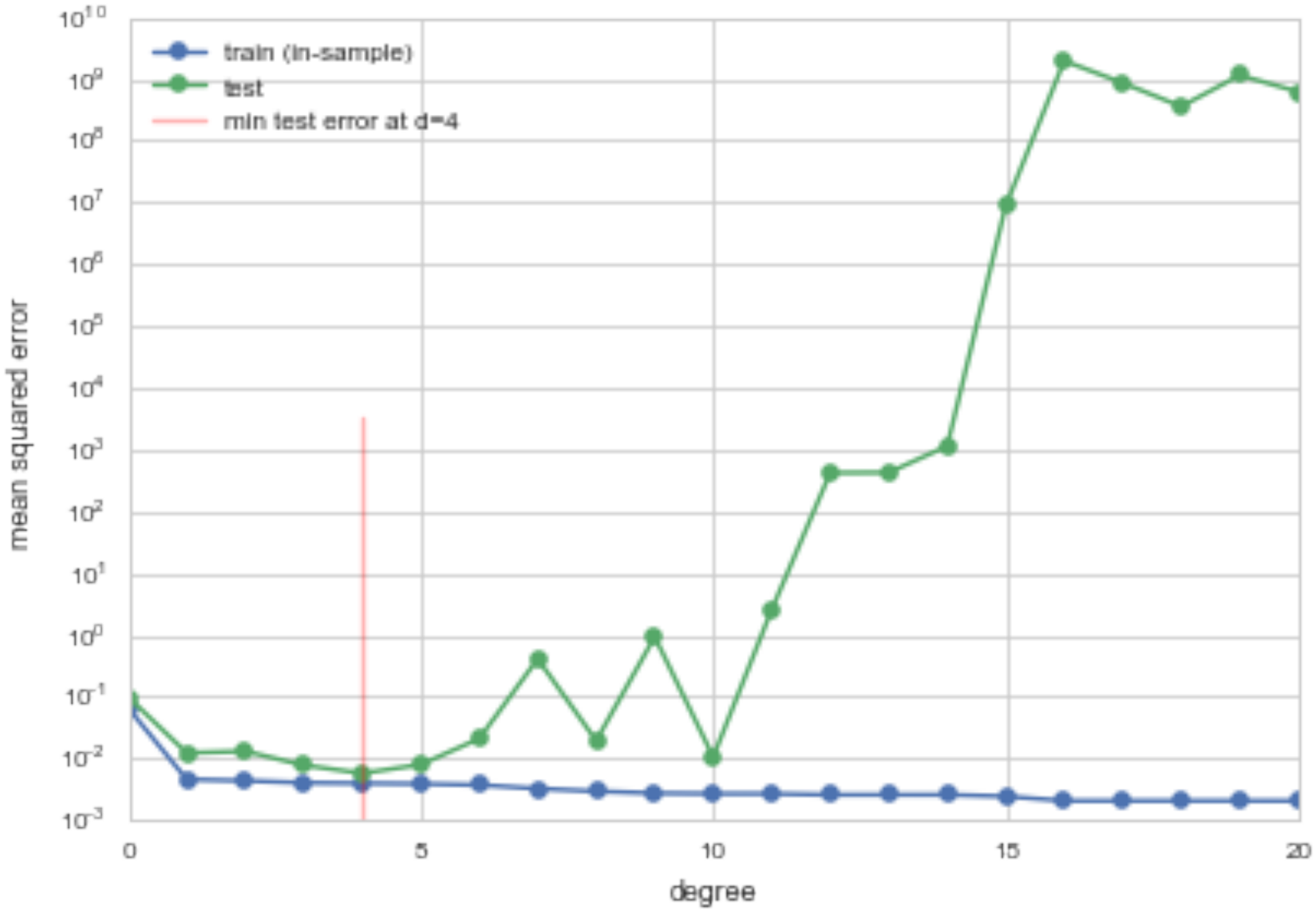



# MODEL COMPARISON: A Large World approach



# We "fit" for d


train (in-sample)
test
min test error at d=4
mean squared error
degree
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 $\mu$, sample drawn with replacement, fraction $\nu$:

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

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

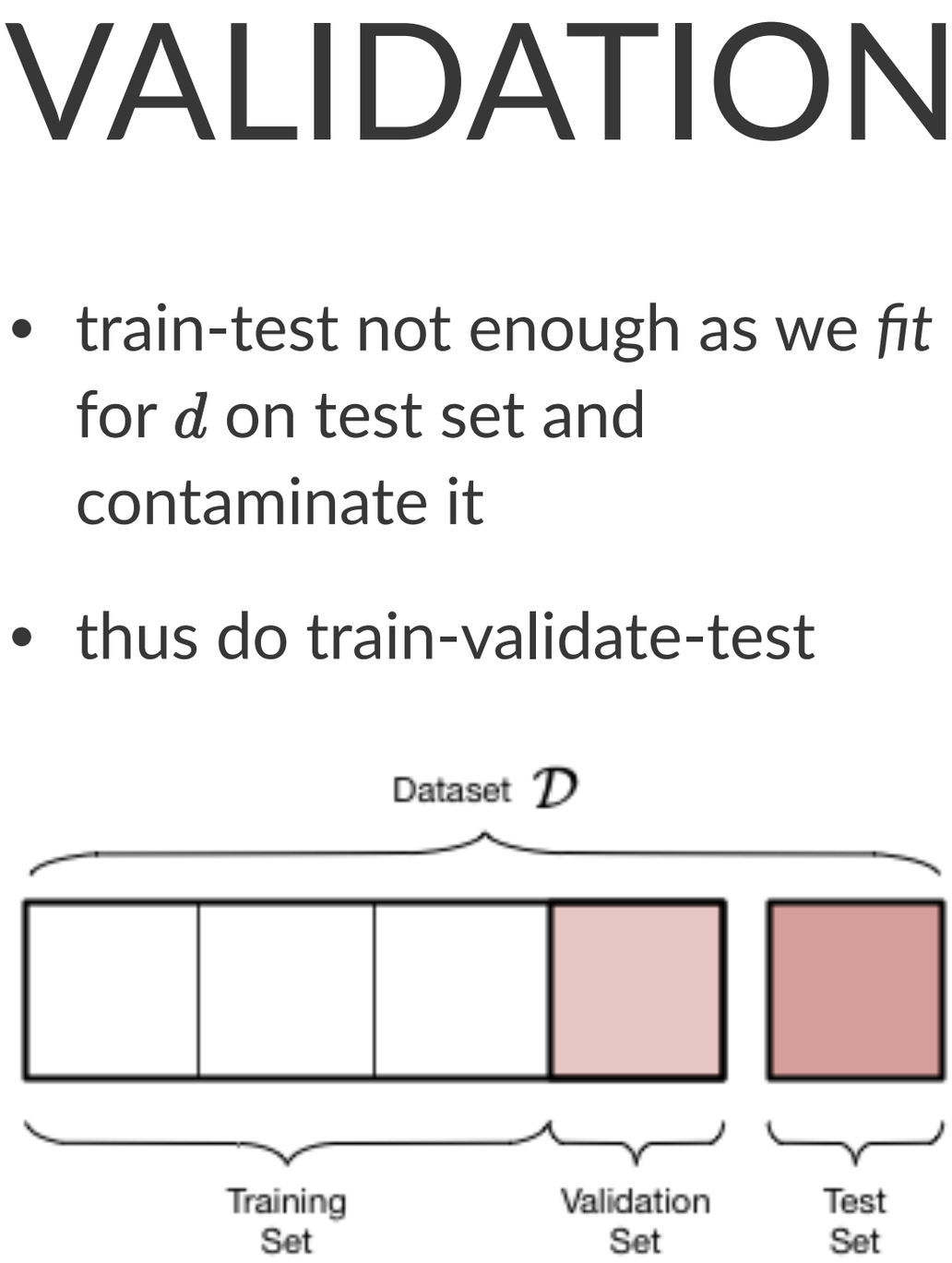
$$P(|R_{in}(h) - R_{out}(h)| > \epsilon) \leq 2e^{-2\epsilon^2 N}$$

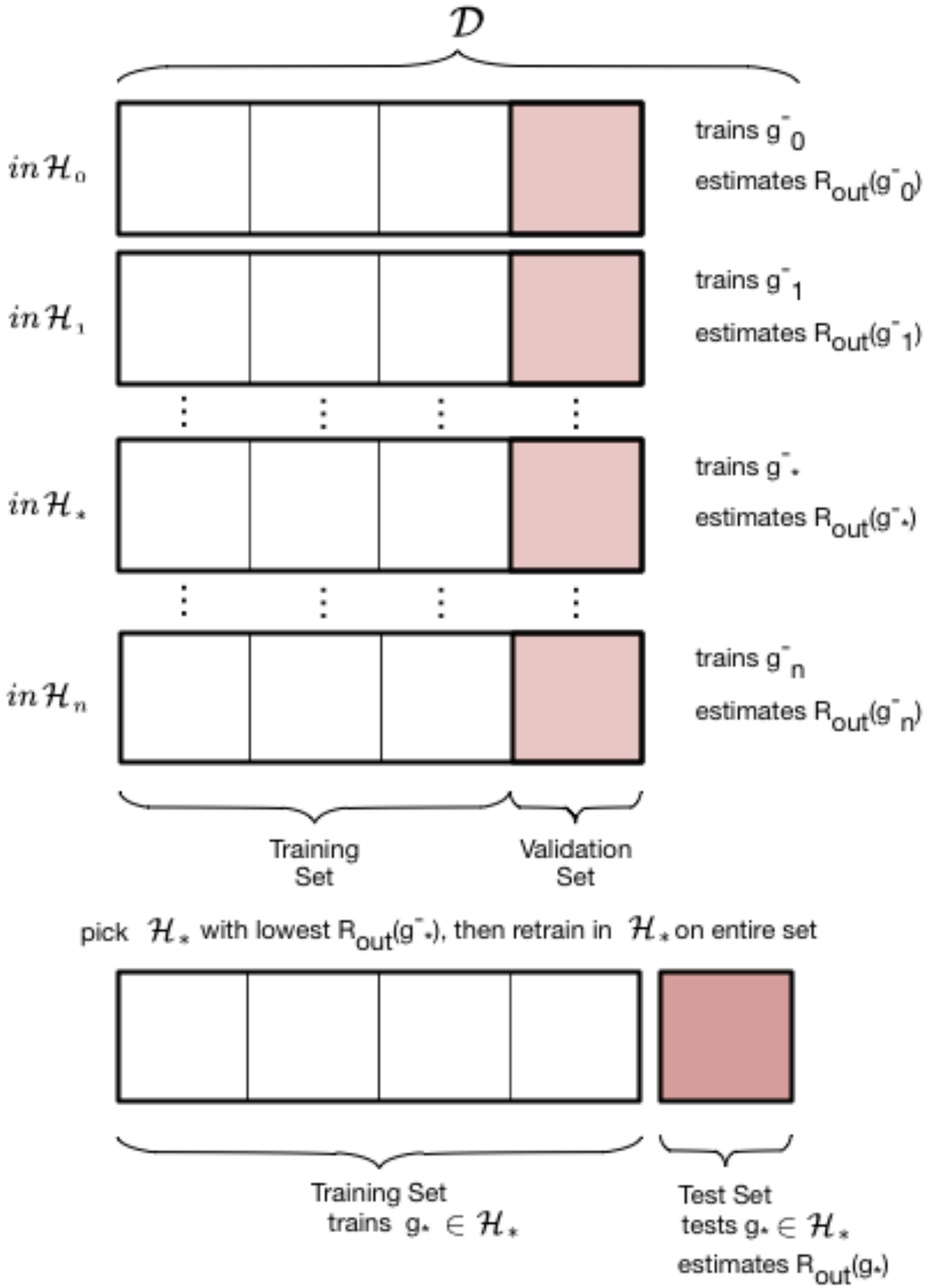
- Hoeffding inequality holds ONCE we have picked a hypothesis $h$, as we need it to label the 1 and 0s.
- But over the training set we one by one pick all the models in the hypothesis space
- best fit $g$ is among the $h$ in $\mathcal{H}$, $g$ must be $h_1$ OR $h_2$ OR....Say **effectively** M such choices:

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

# VALIDATION

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



## usually we want to fit a hyperparameter

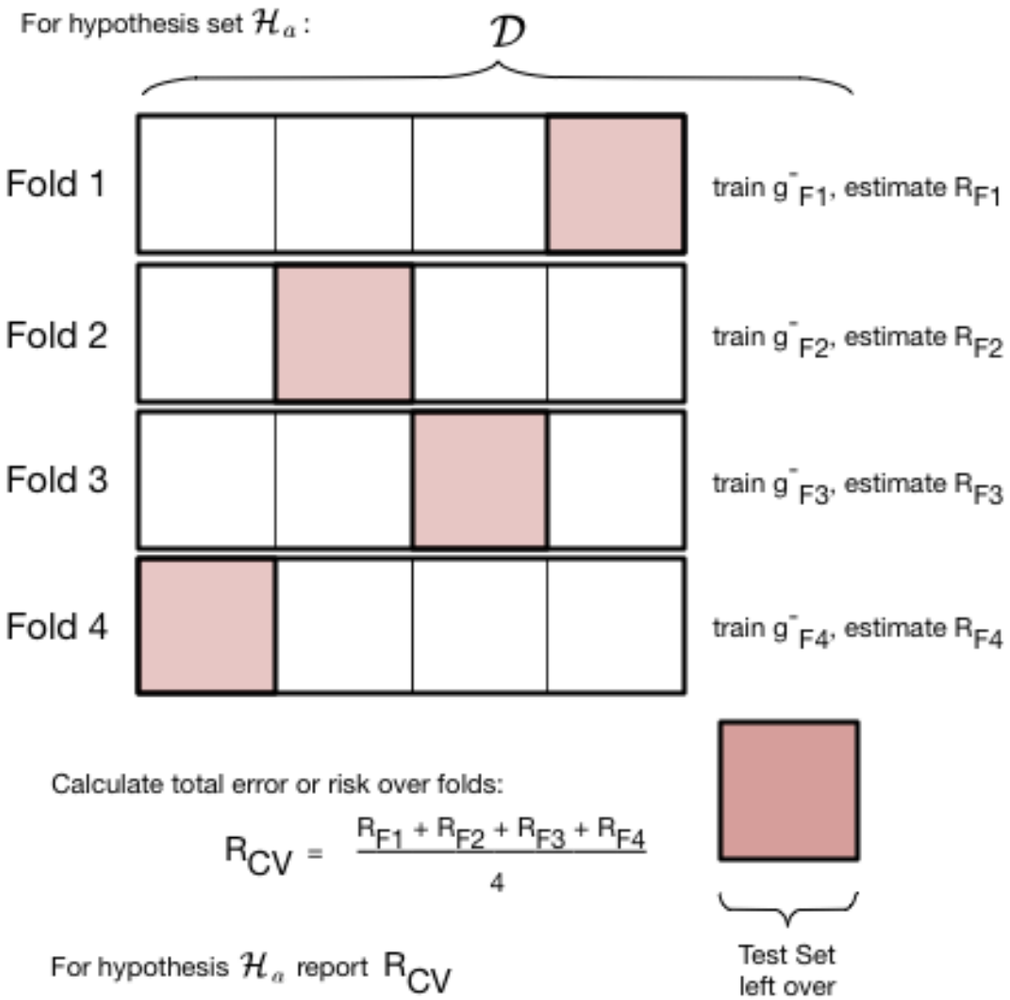
- we **wrongly** already attempted to fit $d$ on our previous test set.
- choose the $d, g^*$ combination with the lowest validation set risk.
- $R_{val}(g^{-*}, d^*)$ has an optimistic bias since $d$ effectively fit on validation set
- its Hoeffding bound must now take into account the grid-size as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

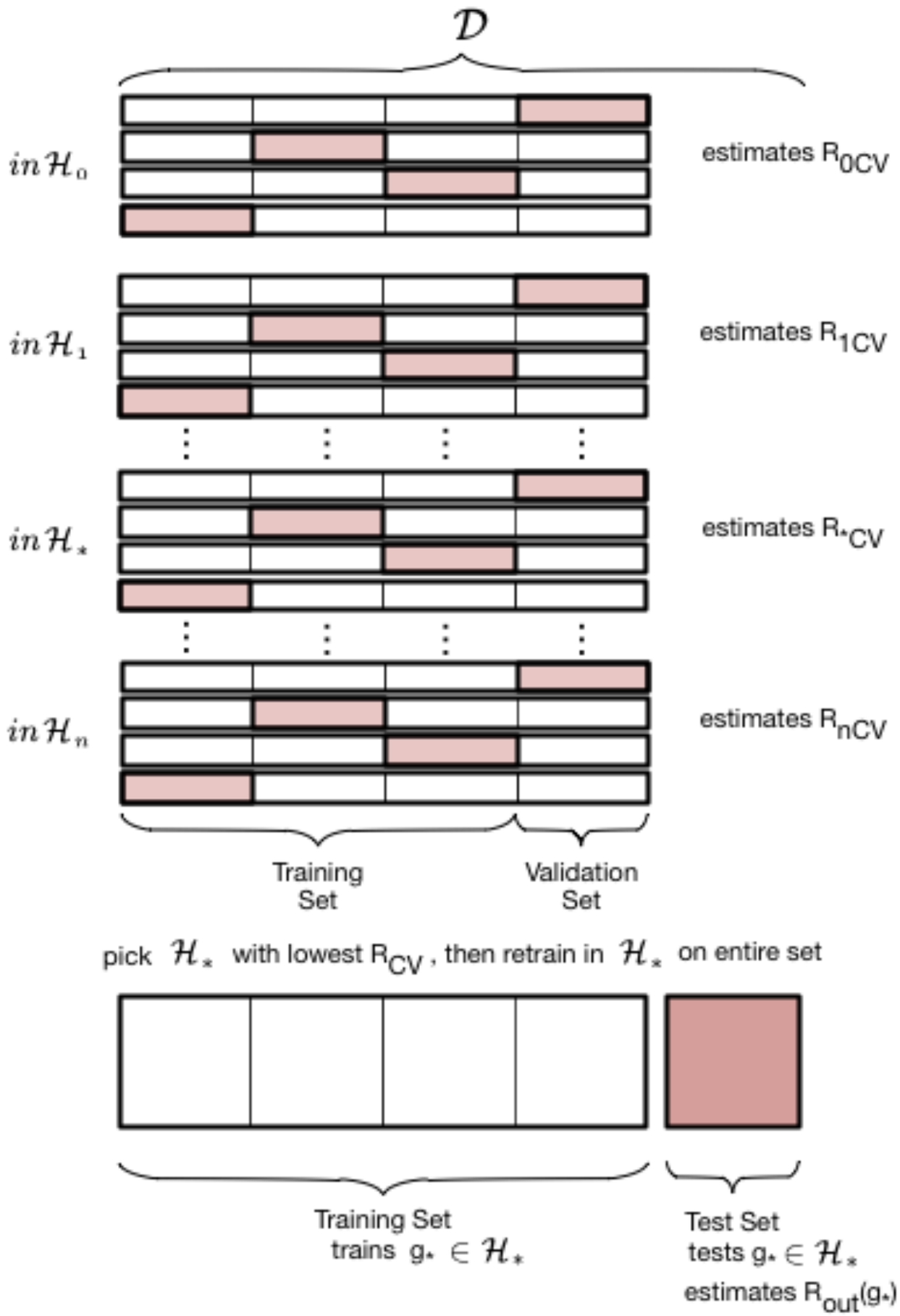
- this size from hyperparameters is typically a smaller size than that from parameters.

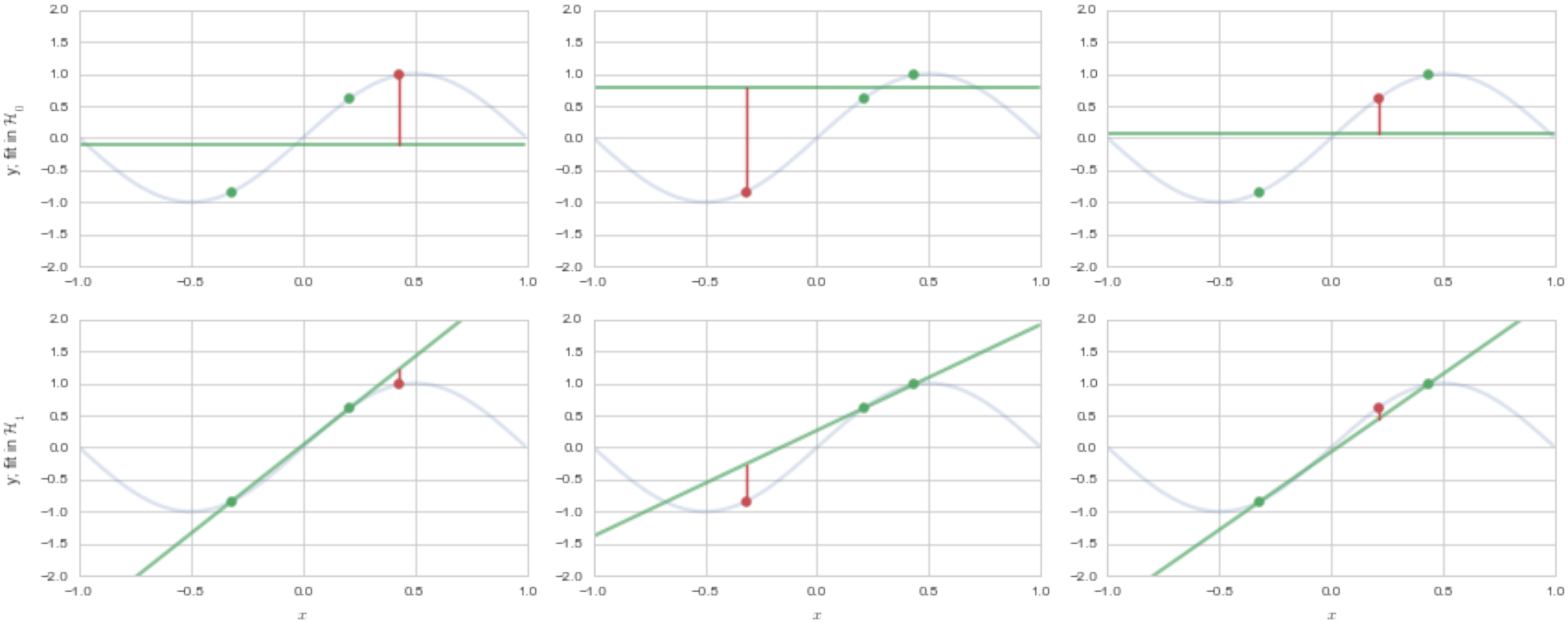
## Retrain on entire set!

- 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



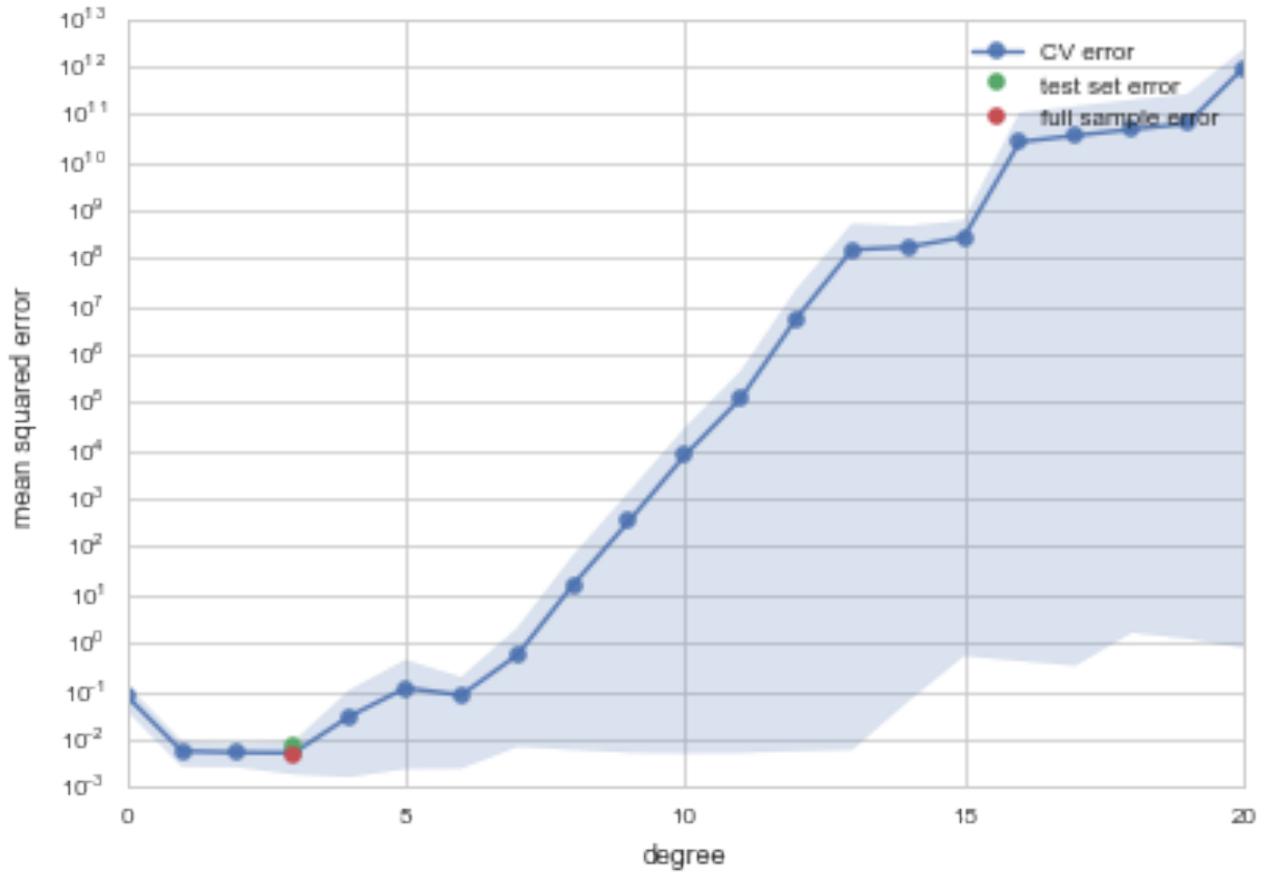

y; fit in $\mathcal{H}_0$
y; fit in $\mathcal{H}_1$
x
x
x

# 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.

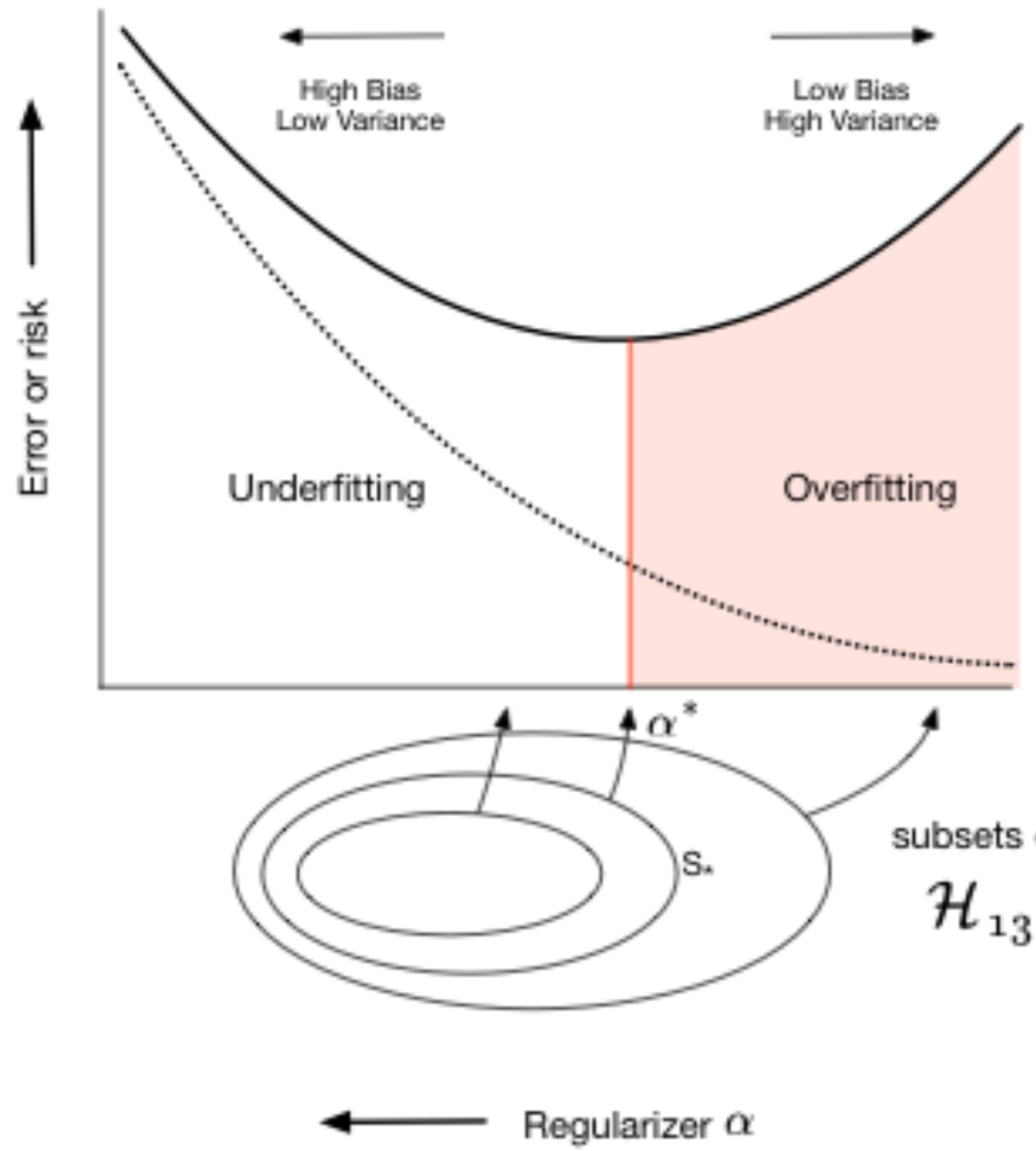
- key subtlety: in the risk averaging process, you are actually averaging over different $g^-$ models, with different parameters.

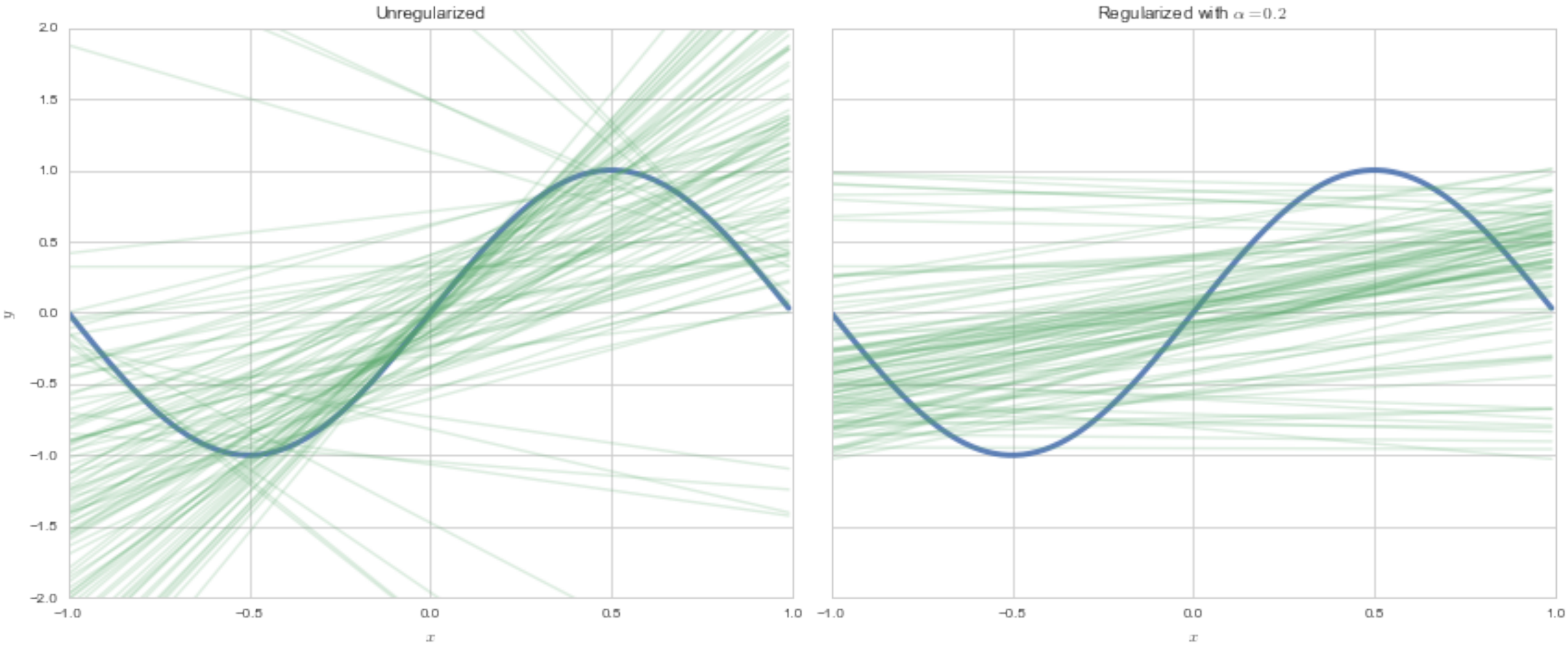
# REGULARIZATION: A SMALL WORLD APPROACH

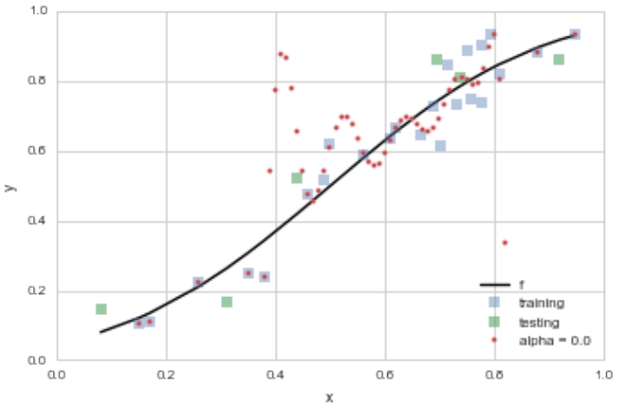
Keep higher a-priori complexity and impose a complexity penalty

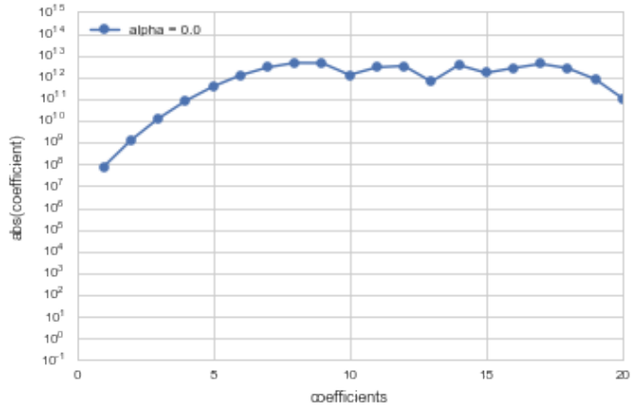
on risk instead, to choose a SUBSET of $\mathcal{H}_{big}$.
We'll make the coefficients small:

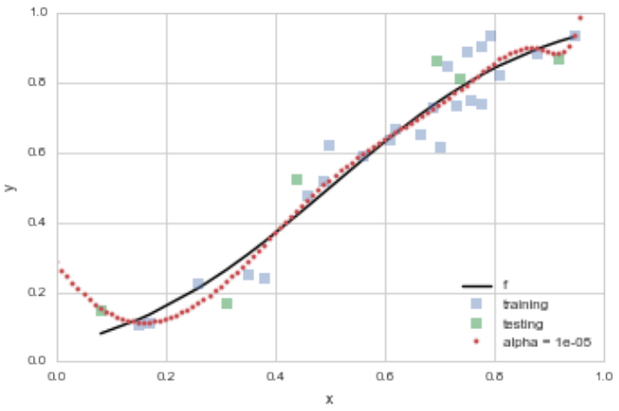
$$\sum_{i=0}^{j} \theta_i^2 < C.$$

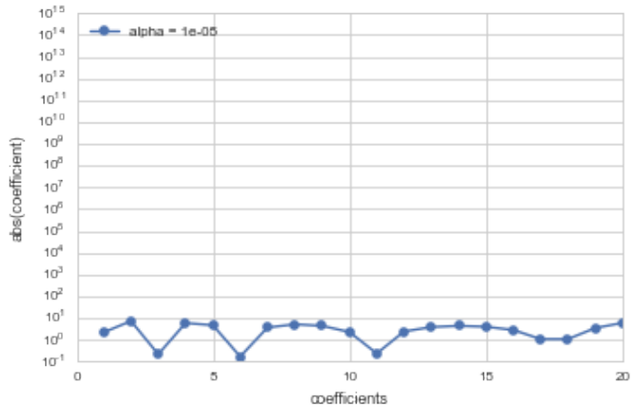


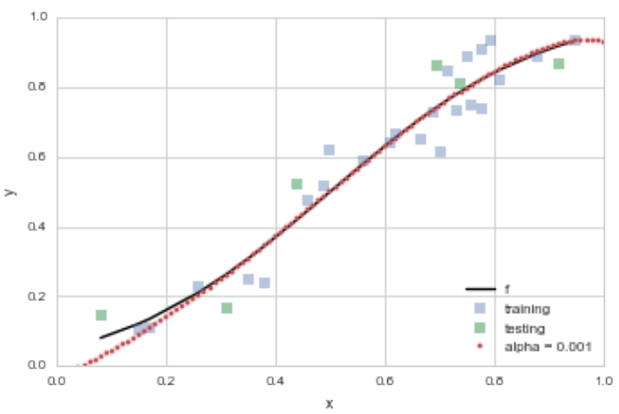

Unregularized
Regularized with $\alpha = 0.2$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
y
−1.0
−0.5
0.0
0.5
1.0
x

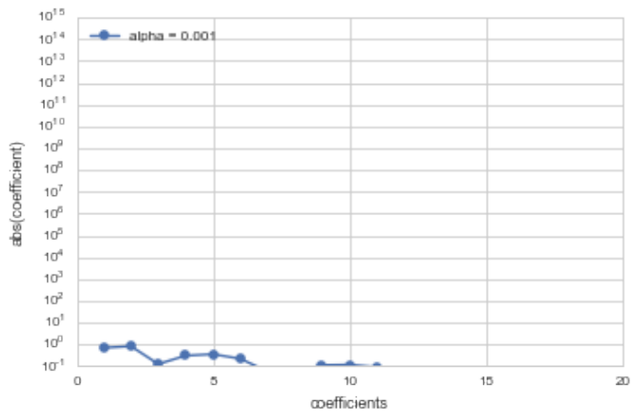


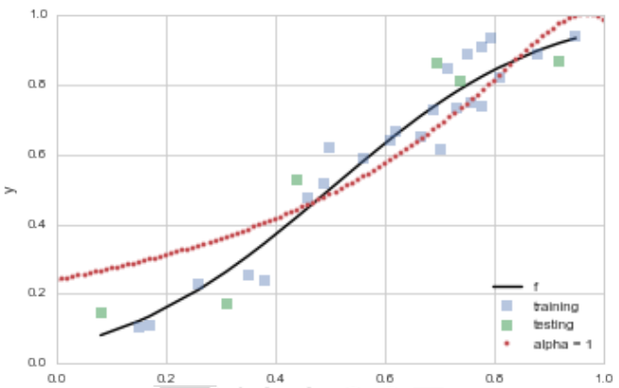



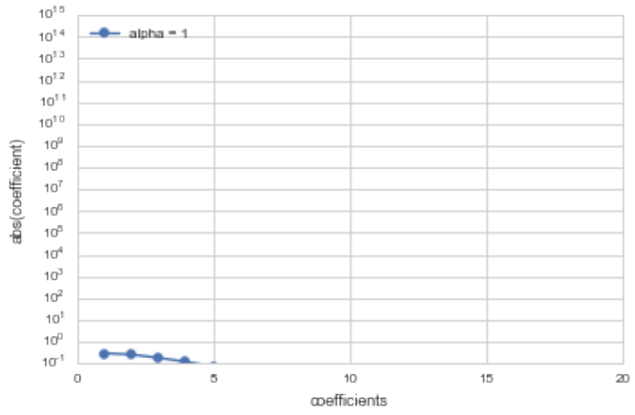





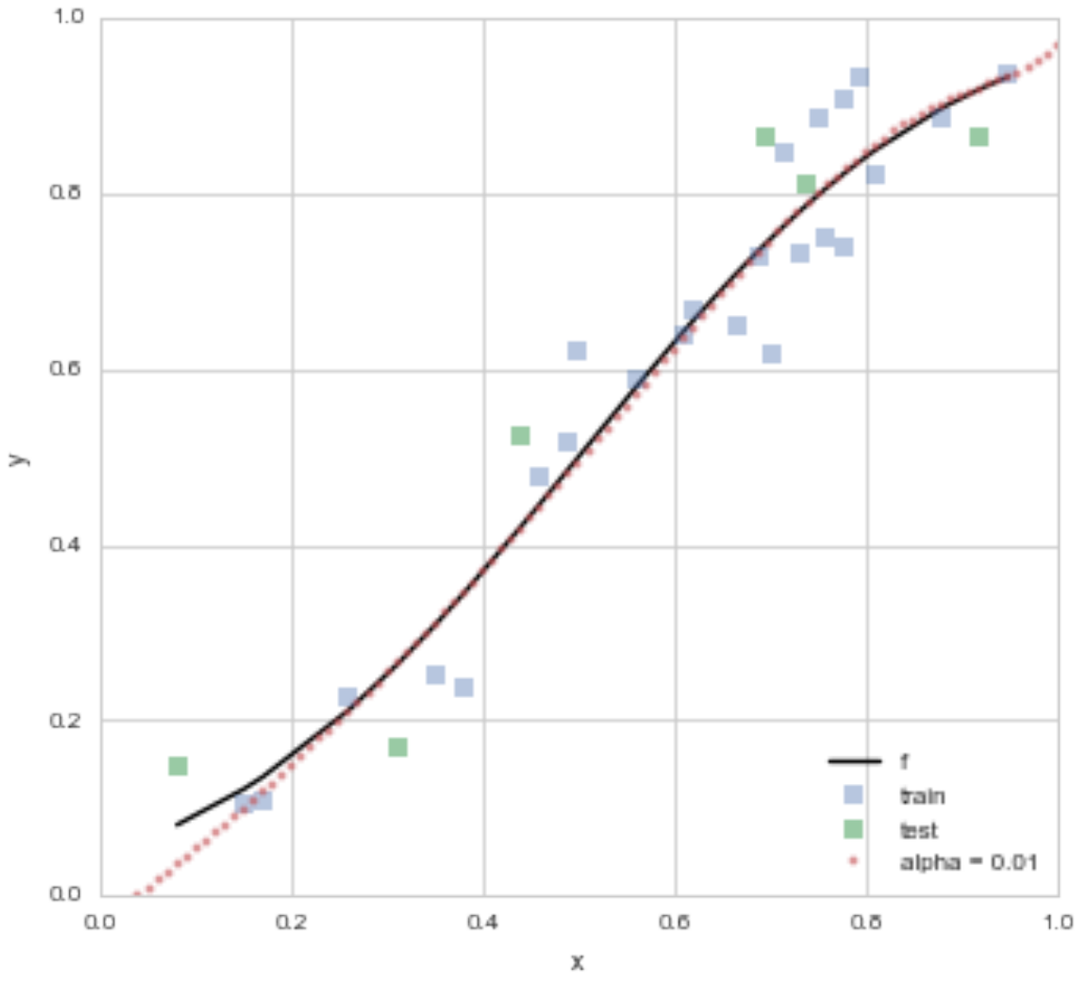

# REGULARIZATION

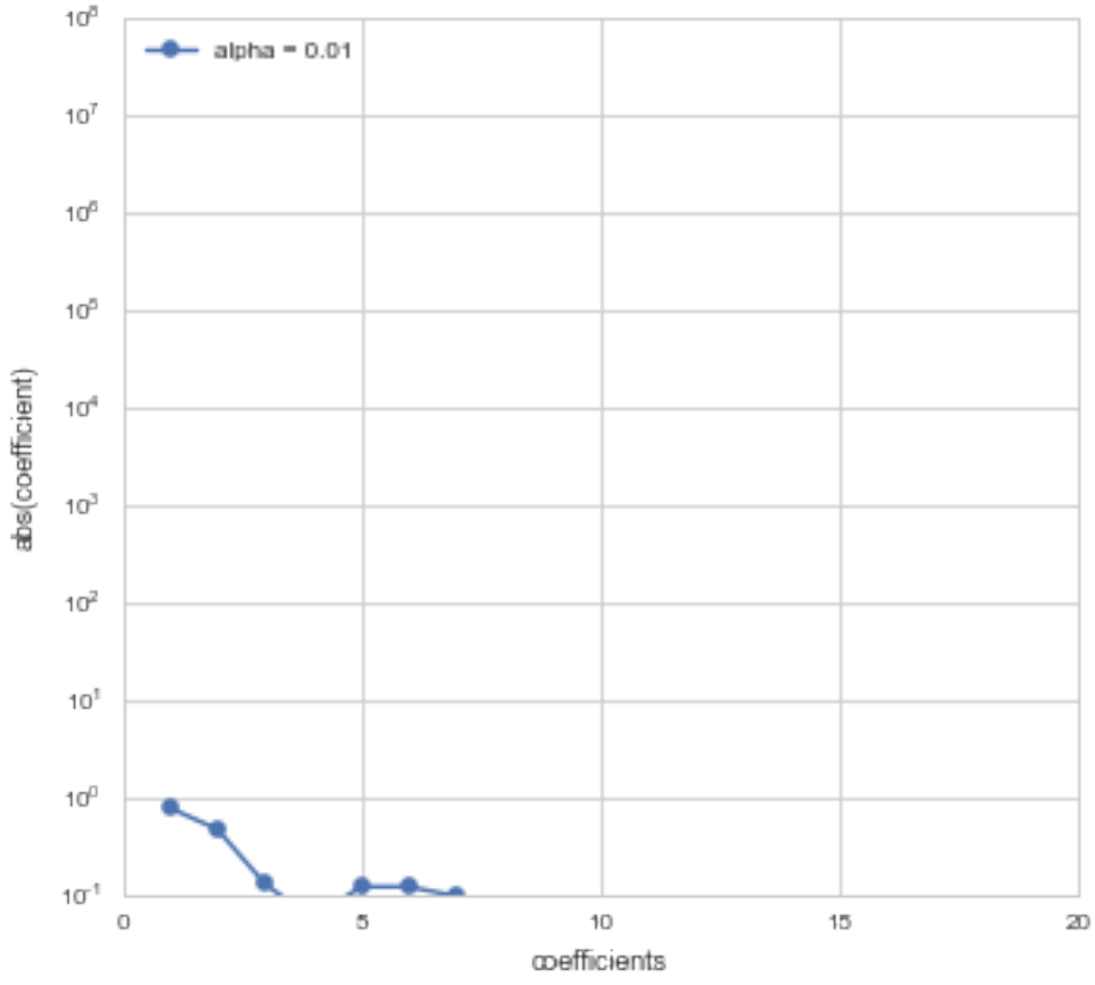
$$\mathcal{R}(h_j) = \sum_{y_i \in \mathcal{D}} (y_i - h_j(x_i))^2 + \alpha \sum_{i=0}^{j} \theta_i^2.$$

As we increase $\alpha$, 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

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

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

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*

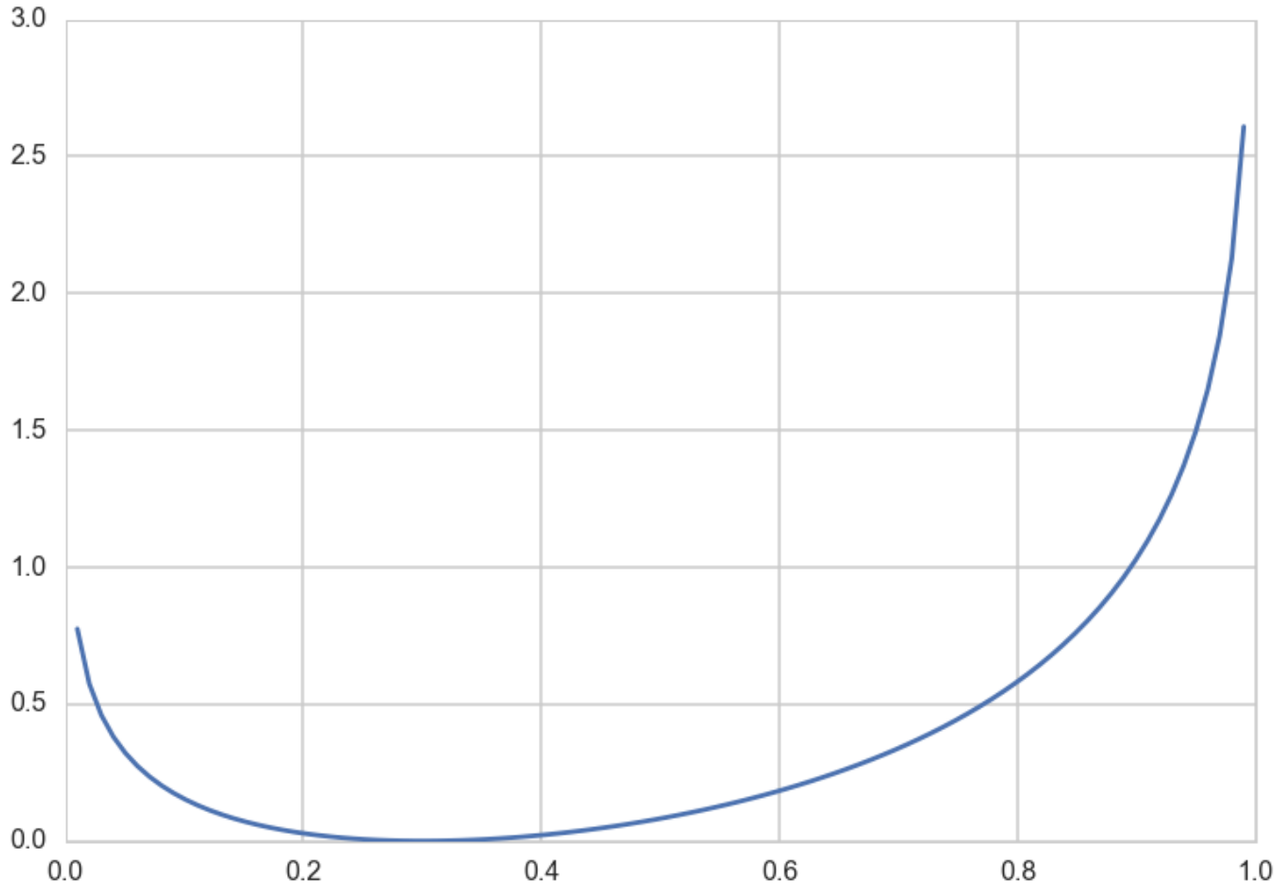
- McElreath page 179

# KL example

Bernoulli Distribution p with $p = 0.3$.

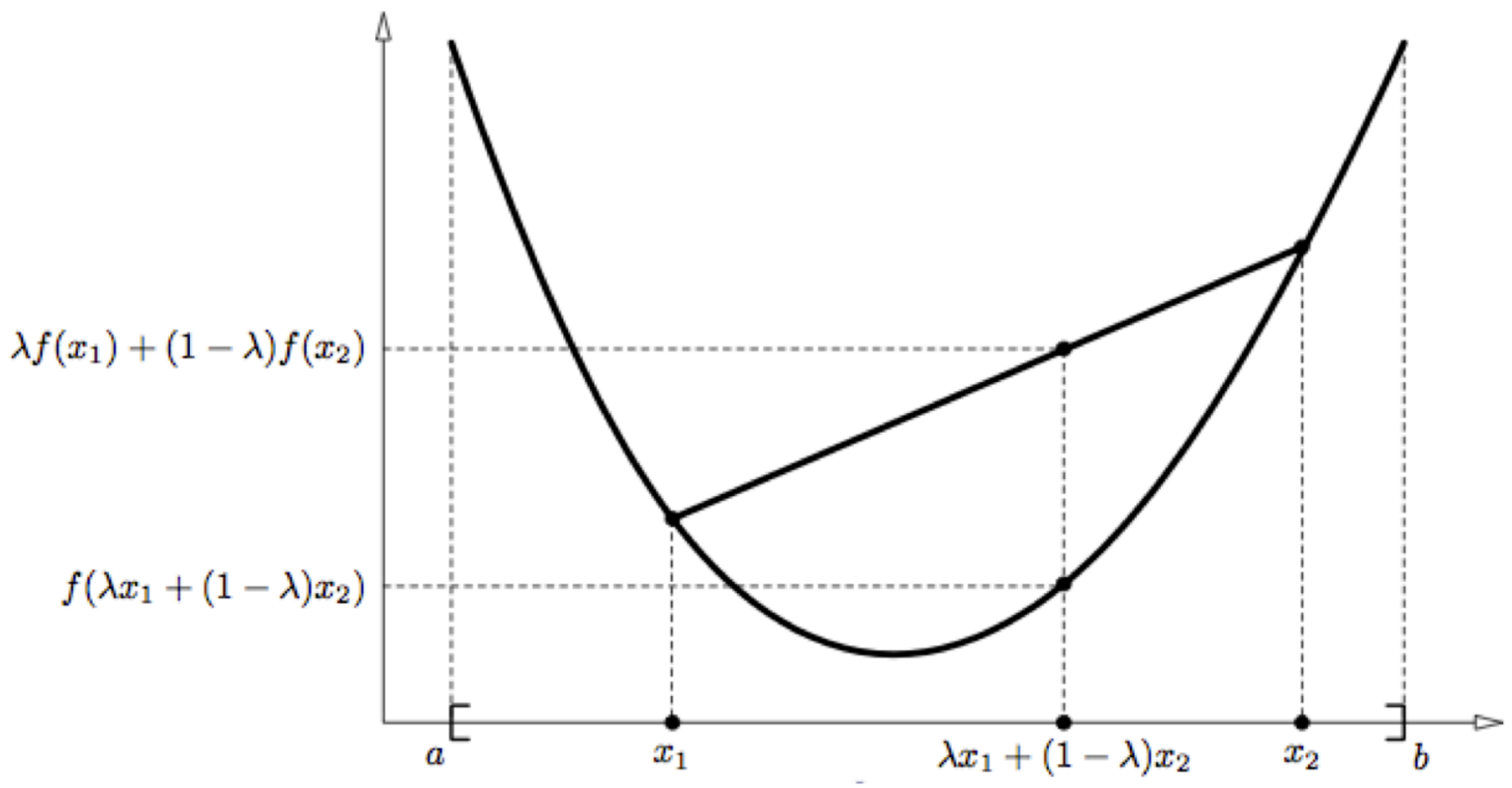
Try to approximate by $q$. What parameter?

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



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

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



# KL-Divergence is always non-negative

Jensen's inequality:

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

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

$$-\log(\int dQ) = 0$$

# 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:

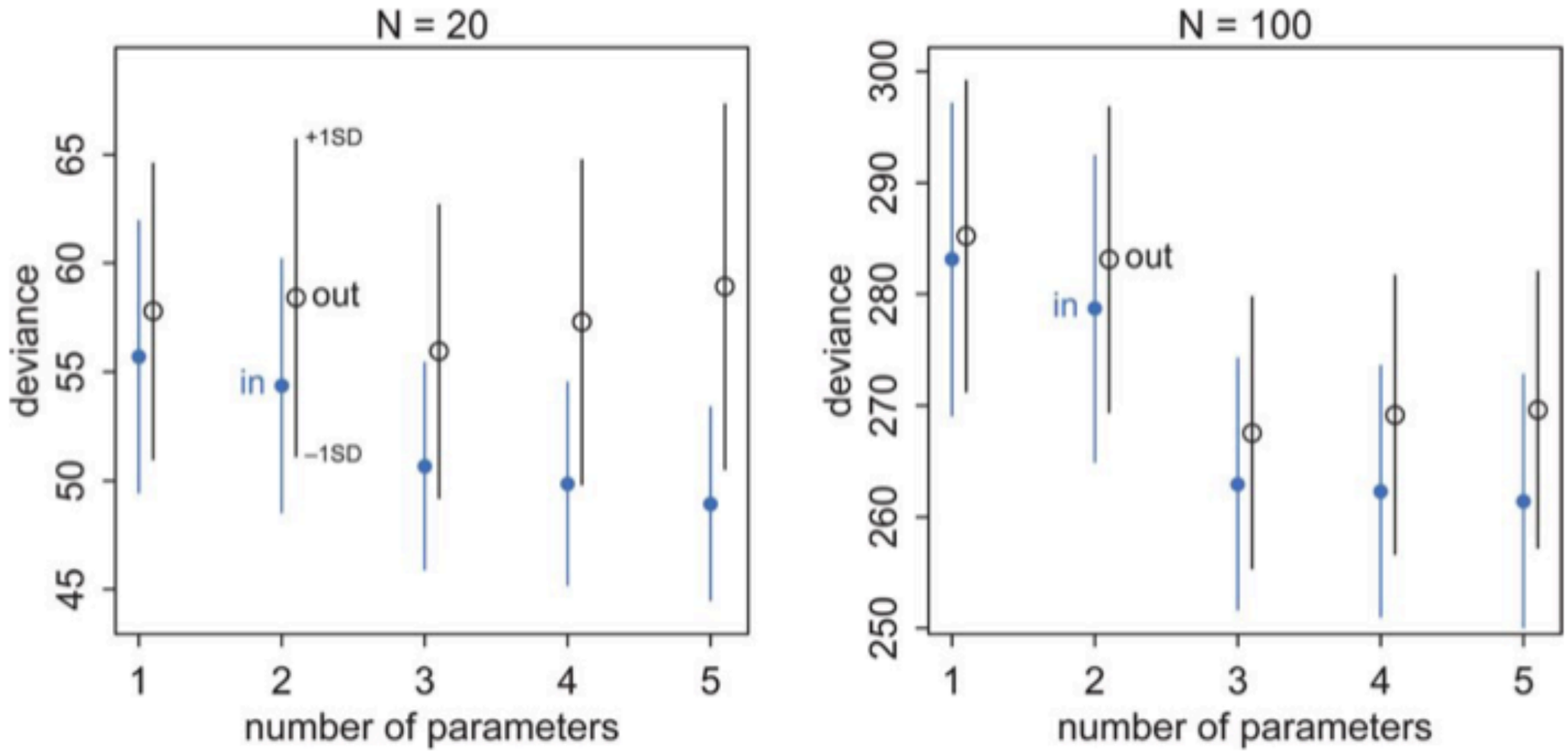
$$\mu_i = 0.15x_{1,i} - 0.4x_{2,i}\,,\;\; y \sim N(\mu, 1)$$

2 parameter model.

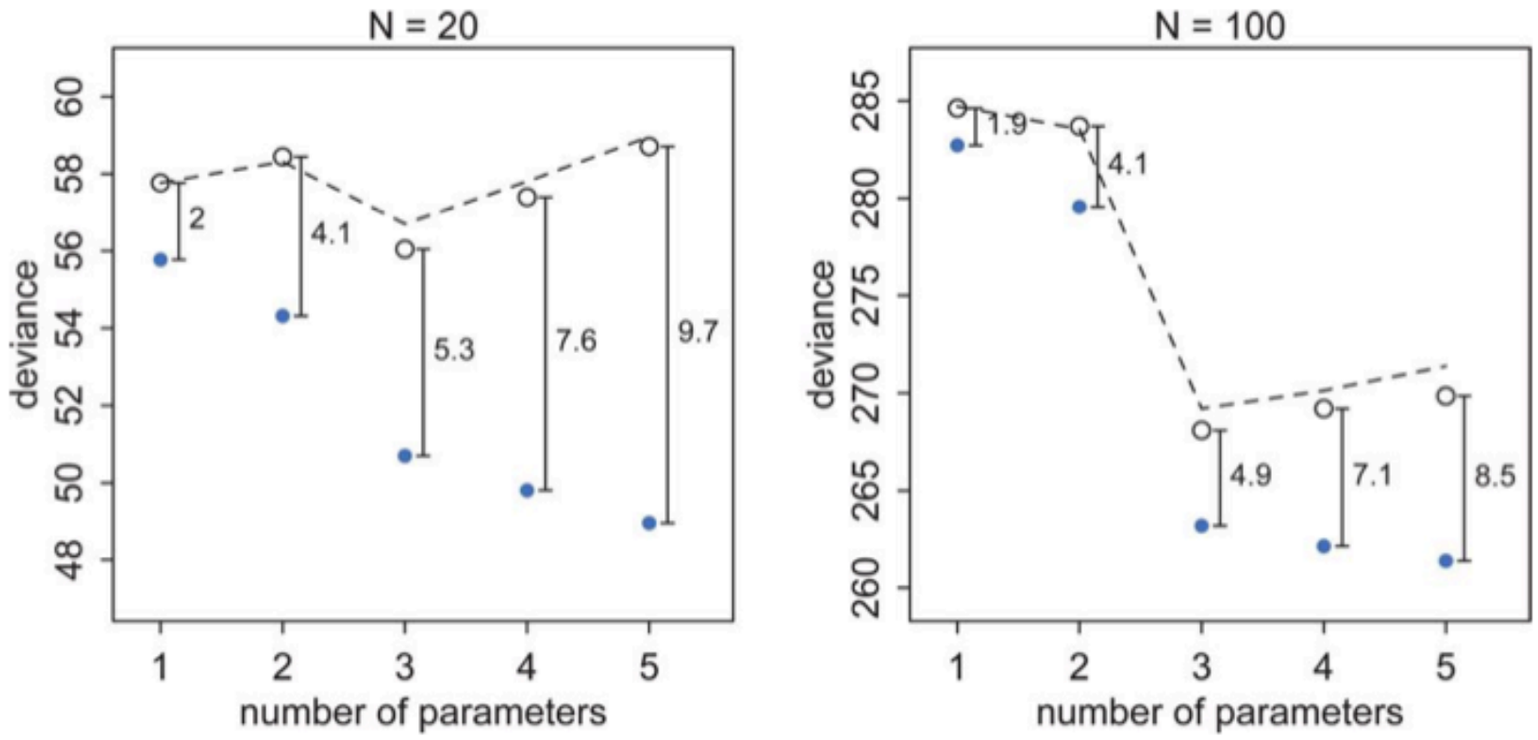
Generate 10,000 realizations, for 1-5 parameters, 20 data points and 100 data points.

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

$$AIC = D_{train} + 2p \text{ where}$$
$$D(q) = -2\sum_i log(q_i) = -2\ell$$

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

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

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