Lecture 6

Risk and Information Theory

AM 207

Last Time:

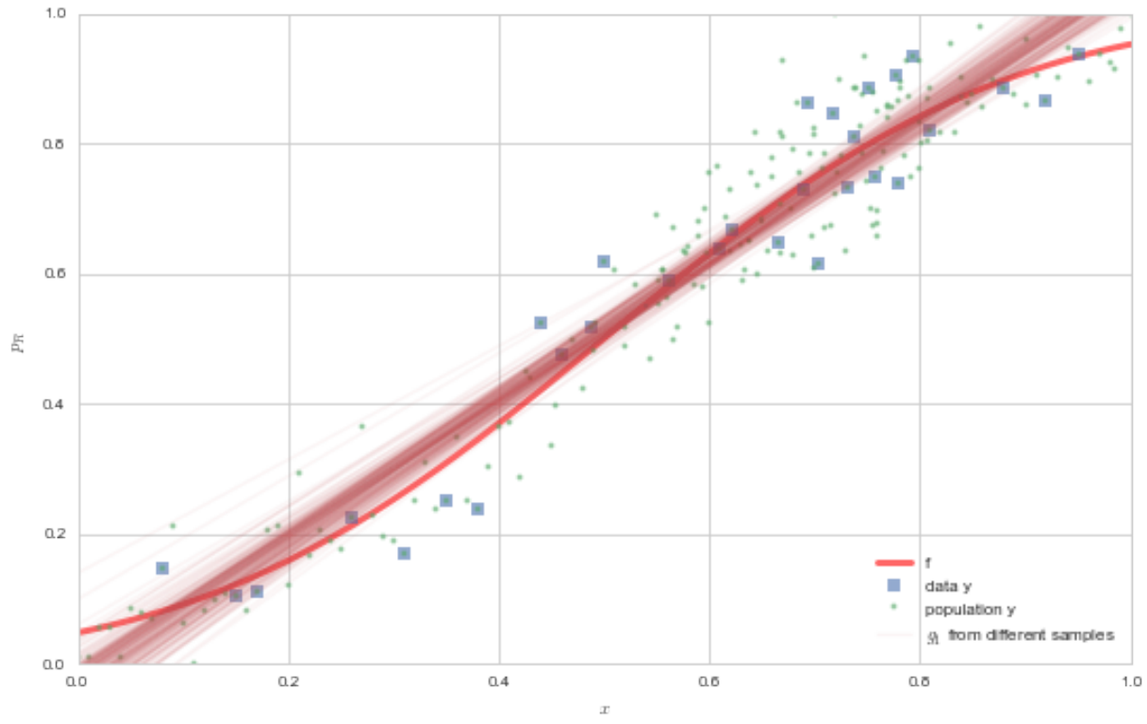
- Normal MLE and Regression
- Test Sets
- Validation and X-validation
- Regularization

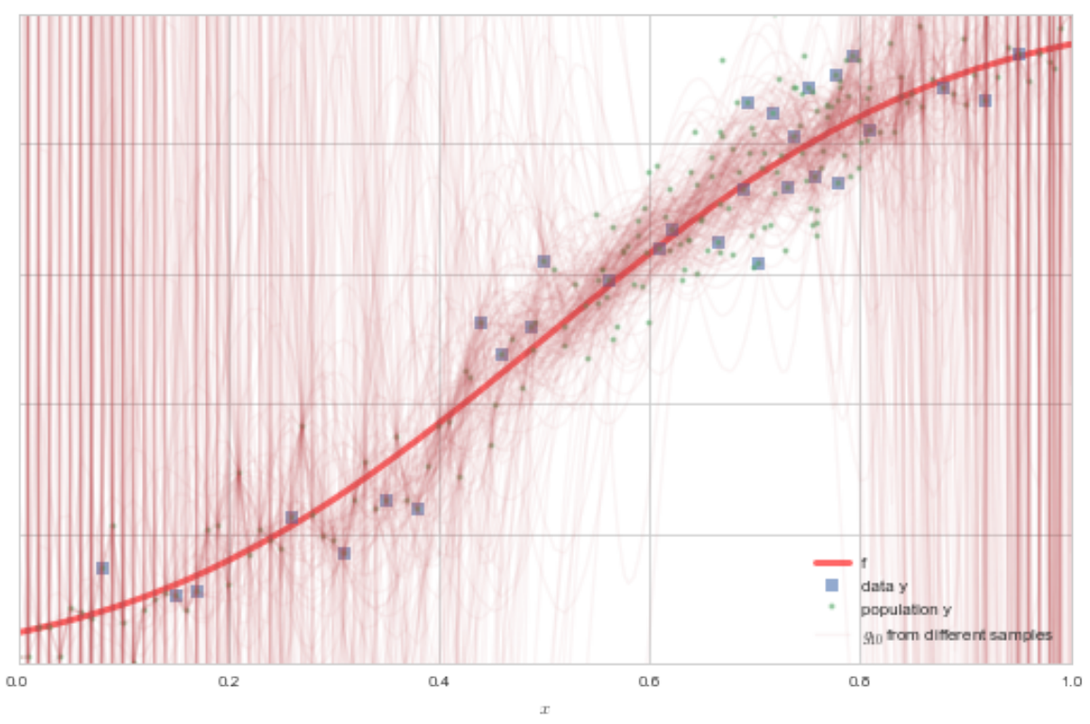
Today

- Risk and Bayes Risk
- The KL Divergence and Deviance
- In-sample penalties: the AIC
- Entropy
- Maximum Likelihood and Entropy

UNDERFITTING (Bias)

vs OVERFITTING (Variance)





Sources of Variability

- sampling (induces variation in a mis-specified model)
- noise (the true $p(y|x)$)
- mis-specification

generate : X^2

fit : X^2

generate : x^2

fit : x

	fixed x	sample x
no ϵ	no $p(y\|x)$	no $p(y\|x)$
	no $p(y\|x)$	$p(y\|x)$ only from sampling ← deterministic noise contribute to variance
ϵ	$p(y\|x)$ only from ϵ	$p(y\|x)$ from both.
	$p(y\|x)$ only from ϵ	$p(y\|x)$ from both.

Risk for a given h

Define:

$$R_{out}(h) = E_{p(x,y)}[(h(x) - y)^2 | h] = \int dydx\, p(x,y)(h(x) - y)^2$$

$$= \int dydx p(y \mid x) p(x)(h(x) - y)^2 = E_X E_{Y|X}[(h - y)^2].$$

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

(we assume 0 mean finite-variance noise ϵ)

- Varying training sets make empirical $R_{out}(h)$ a stochastic quantity, varying from one training set to another.
- This can be written as:

$$R_{out}(\hat{h}_n) = E_{p(x,y)}[(h(x) - y)^2 \mid \hat{h}_n]$$
$$= \int dx p(x,y)(\hat{h}_n(x) - y)^2.$$

- Average empirical risk over the training sets (a different model is fit on each set)

Bayes Risk

$$R^* = \inf_h R_{out}(h) = \inf_h \int dx p(x,y)(h(x)-y)^2.$$

Its the minimum risk **ANY** model can achieve.

Want to get as close to it as possible.

Could infimum amongst all possible functions. OVERFITTING!

Instead restrict to a particular Hypothesis Set: $\mathcal{H}$.

Bayes Risk for Regression

$$R_{out}(h) = \int dx p(x,y)(h(x)-y)^2.$$

$$= E_X E_{Y|X}[(h-y)^2] = E_X E_{Y|X}[(h-r+r-y)^2]$$

where $r(x) = E_{Y|X}[y]$ is the "regression" function.

$$R_{out}(h) = E_X[(h-r)^2] + R^*; R^* = E_X E_{Y|X}[(r-y)^2]$$

```
R* is the non-reducible error by any choice of h,
\sigma^2 coming from noise
```

For 0 mean, finite variance, then, σ^2, the noise of ϵ, is the Bayes Risk, also called the irreducible error.

AM 207

Empirical Risk Minimization

- LLN suggests that we can replace the risk integral by a data sum and then minimize
- Assume $(x_i, y_i) \sim P(x, y)$ (use empirical distrib)
- Fit hypothesis $h = g_{\mathcal{D}}$, where $\mathcal{D}$ is our training sample.
- $R_{out}(g_{\mathcal{D}}) = \sum_{i \in \mathcal{D}} (g_i - y_i)^2$
- minimize to get best for $g_{\mathcal{D}}$

$$R(h) = E_{XY}[L(h, y)]$$

$$\hat{R}_n = \frac{1}{N} \sum_i L(y_i, h(x_i))$$

For each h LLN implies convergence from empirical to actual.

Now, $R^* = \inf_{allh} R(h)$ becomes infimum over empirical risks. But again restrict to $\mathcal{H}$ otherwise overfitting!

- Varying training sets make empirical $R_{out}(h)$ a stochastic quantity, varying from one training set to another.
- Thus average empirical risk over the training sets (a different model is fit on each set)
- **Goal of Learning**: Build a function whose risk is closest to Bayes Risk

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

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

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

variance bias irreducible error from noise

where $y = f(x) + \epsilon$ is the true generating process and ϵ has 0 mean and finite variance σ^2.

AM 207

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

This is the bias variance decomposition for regression.

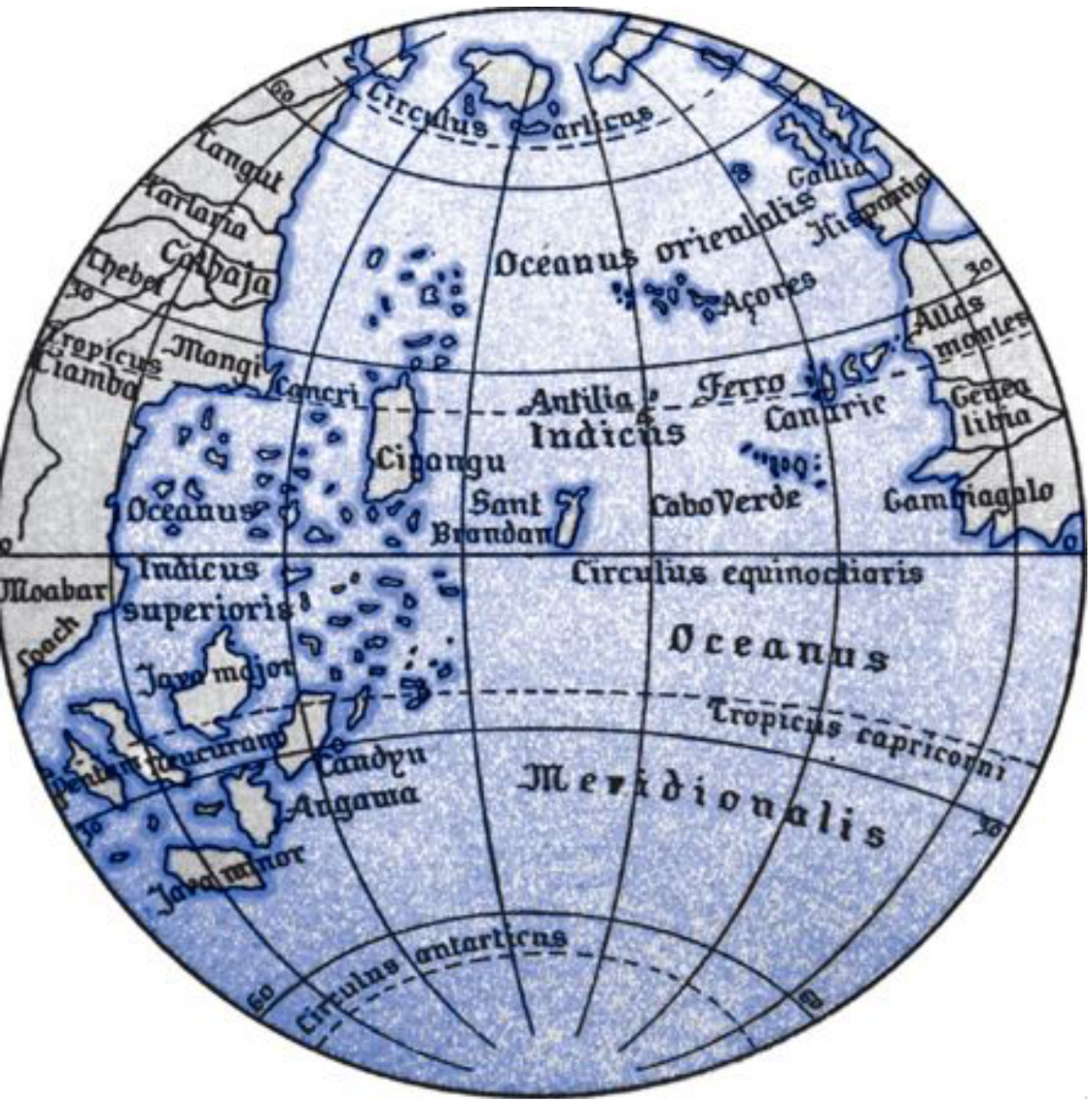
Or, written as $\langle R \rangle - R^*$, this is

$\texttt{variance} + \texttt{bias}^2$, or

$\texttt{estimation-error} + \texttt{approximation-error}$

$$R(g) - \inf_{g \in \mathcal{H}} R(g) + \inf_{g \in \mathcal{H}} R(g) - R^*$$

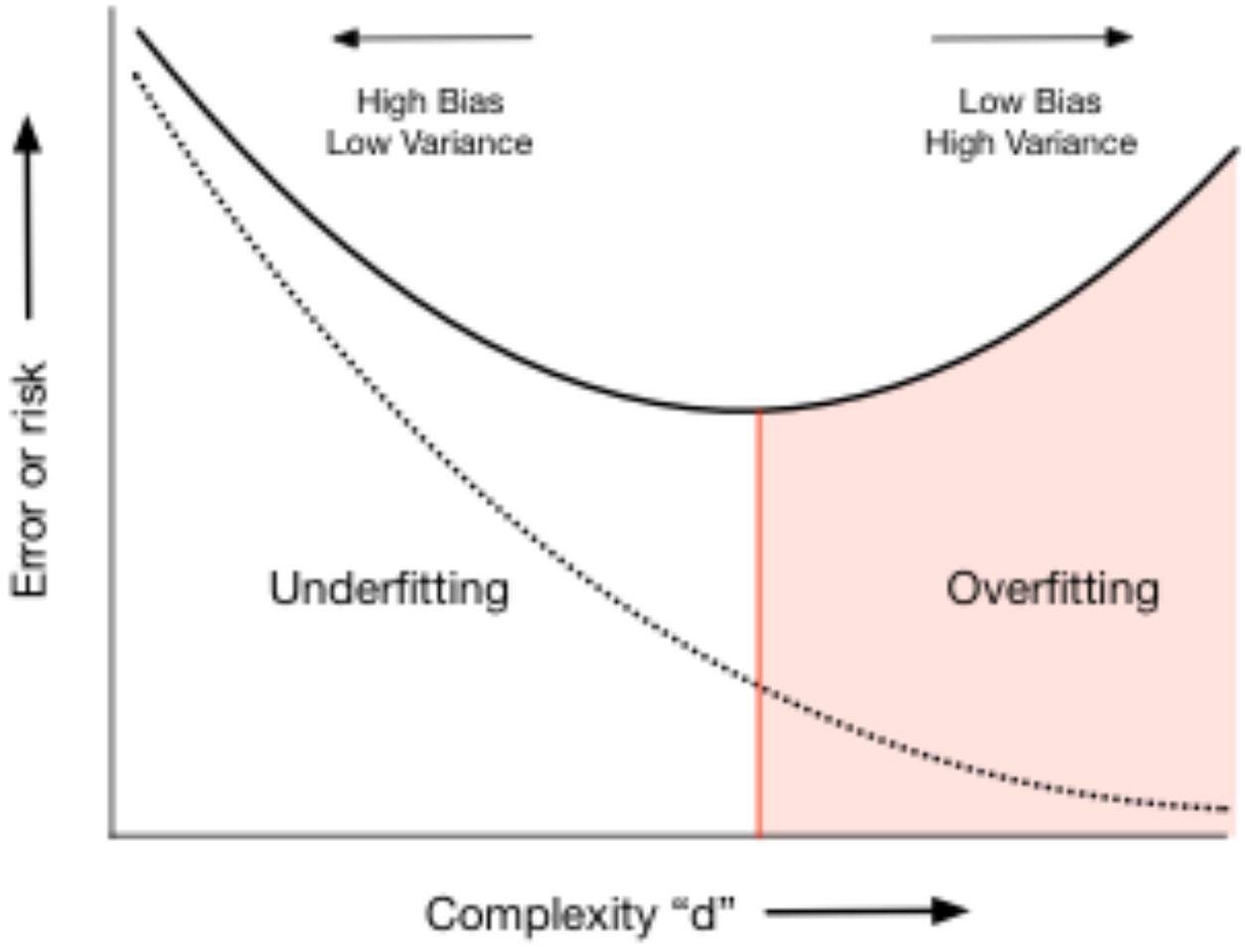
- first term is **variance**, squared error of the various fit g's from the average g, the hairiness.
- second term is **bias**, how far the average g is from the original f this data came from.
- third term is the **stochastic noise**, minimum error that this model will always have.

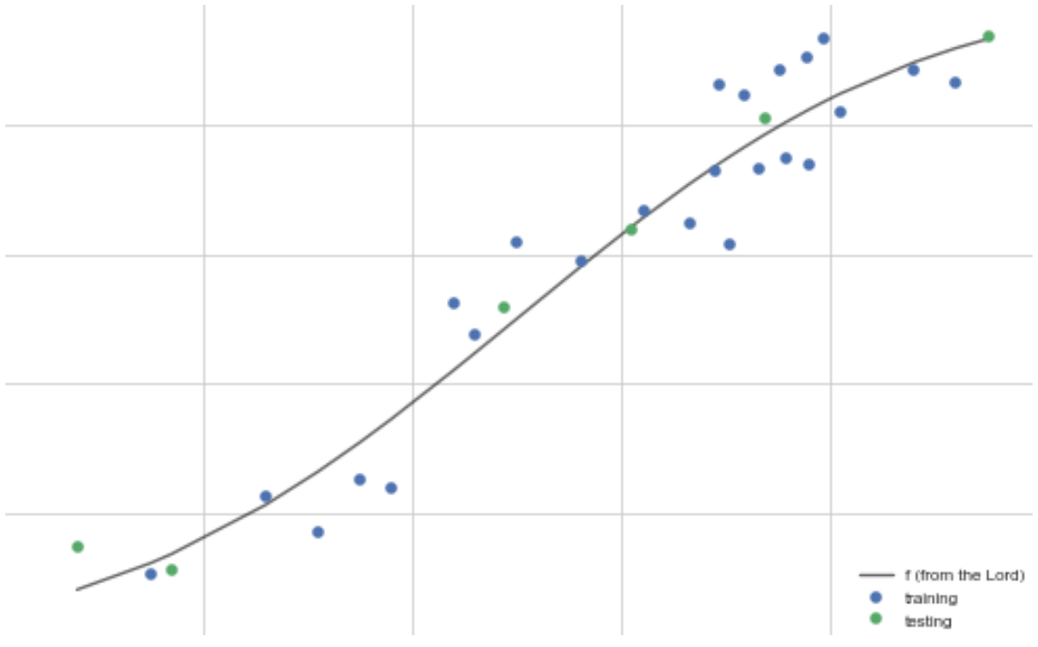


SMALL World vs BIG World

- *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".

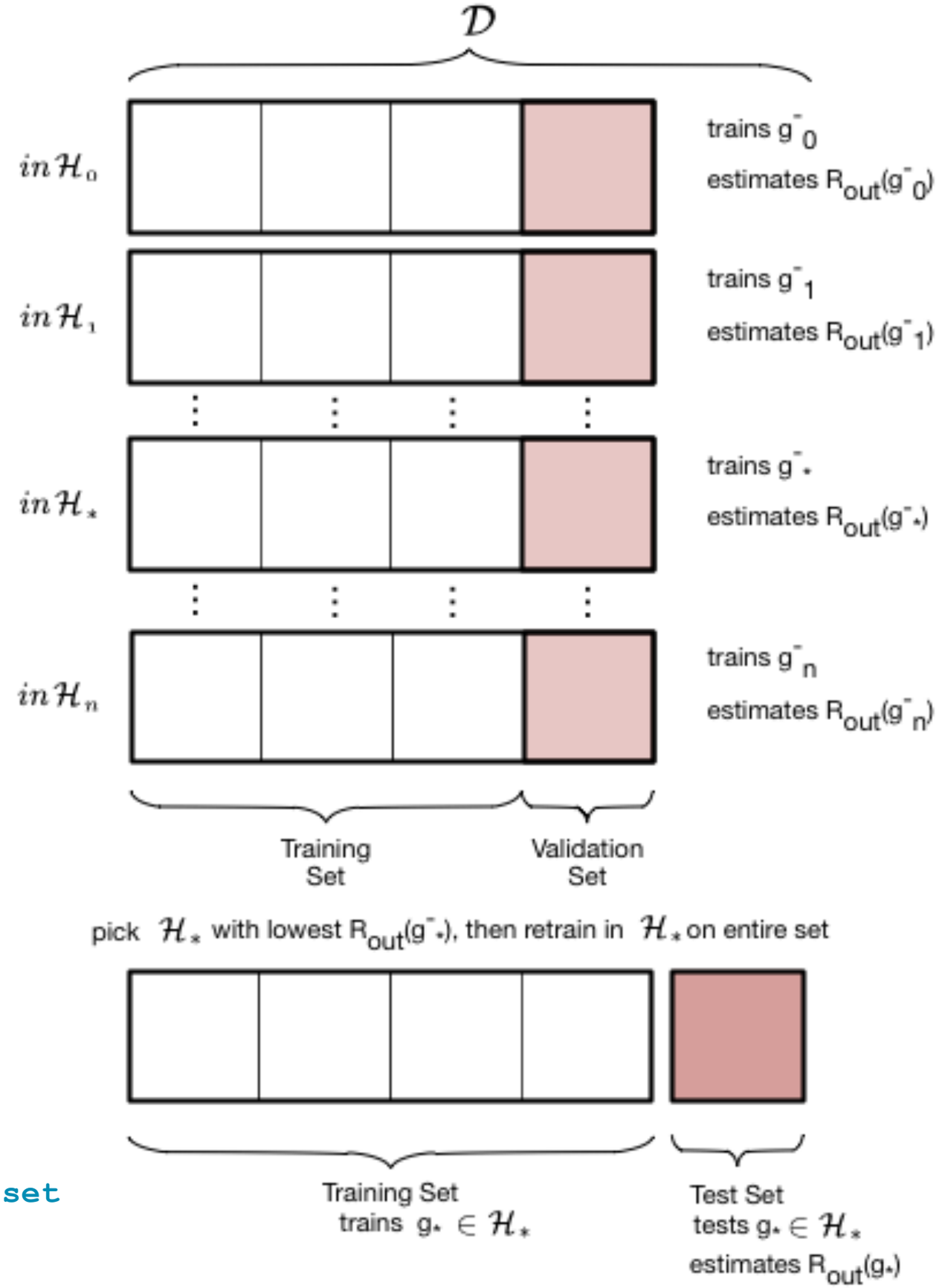
MODEL COMPARISON: A Large World approach





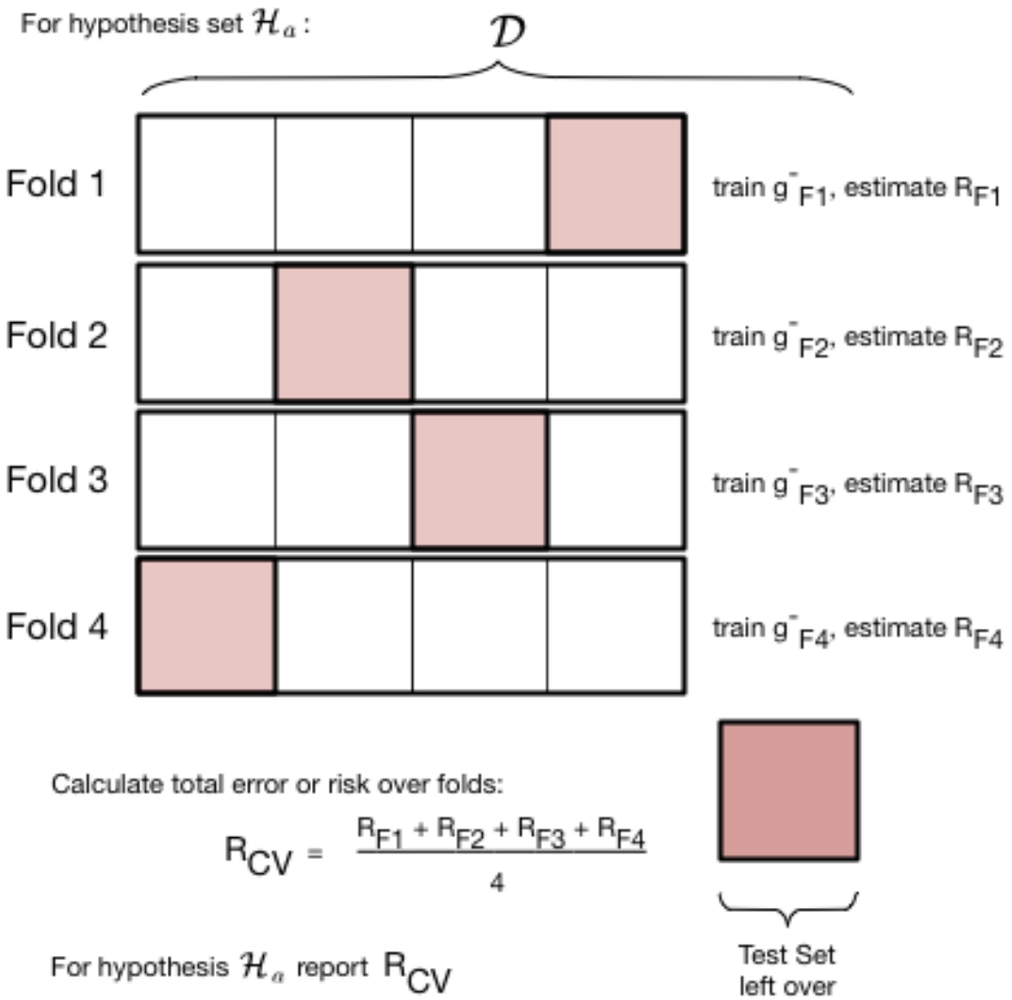
VALIDATION

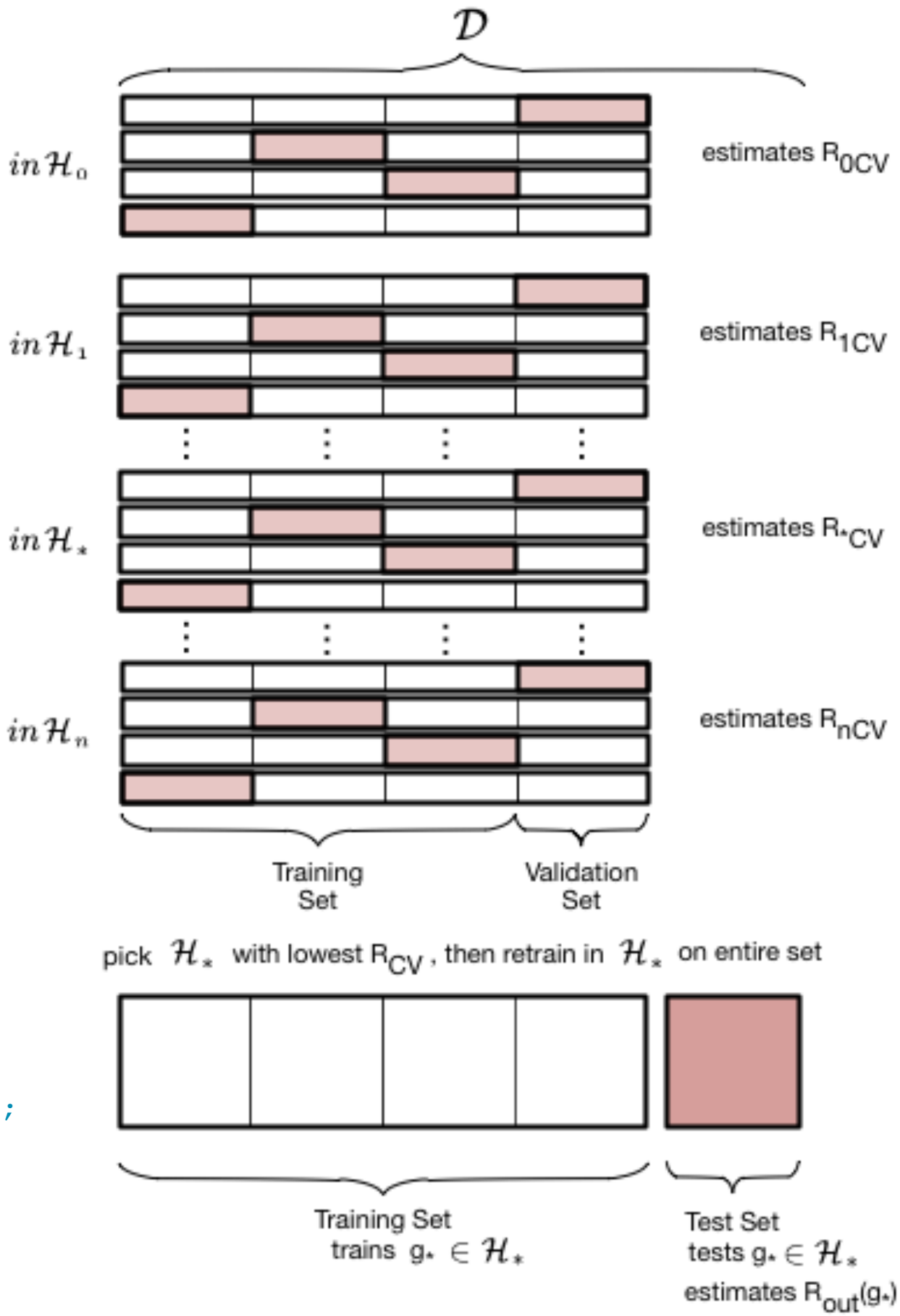
- train-test not enough as we *fit* for d on test set and contaminate it
- thus do train-validate-test



Empirically compute Rout on the validation set

CROSS-VALIDATION





Empirical Rout on different validation sets;
And then compare Rout with the other models
-> other choices of CV parameters

REGULARIZATION: A SMALL WORLD APPROACH

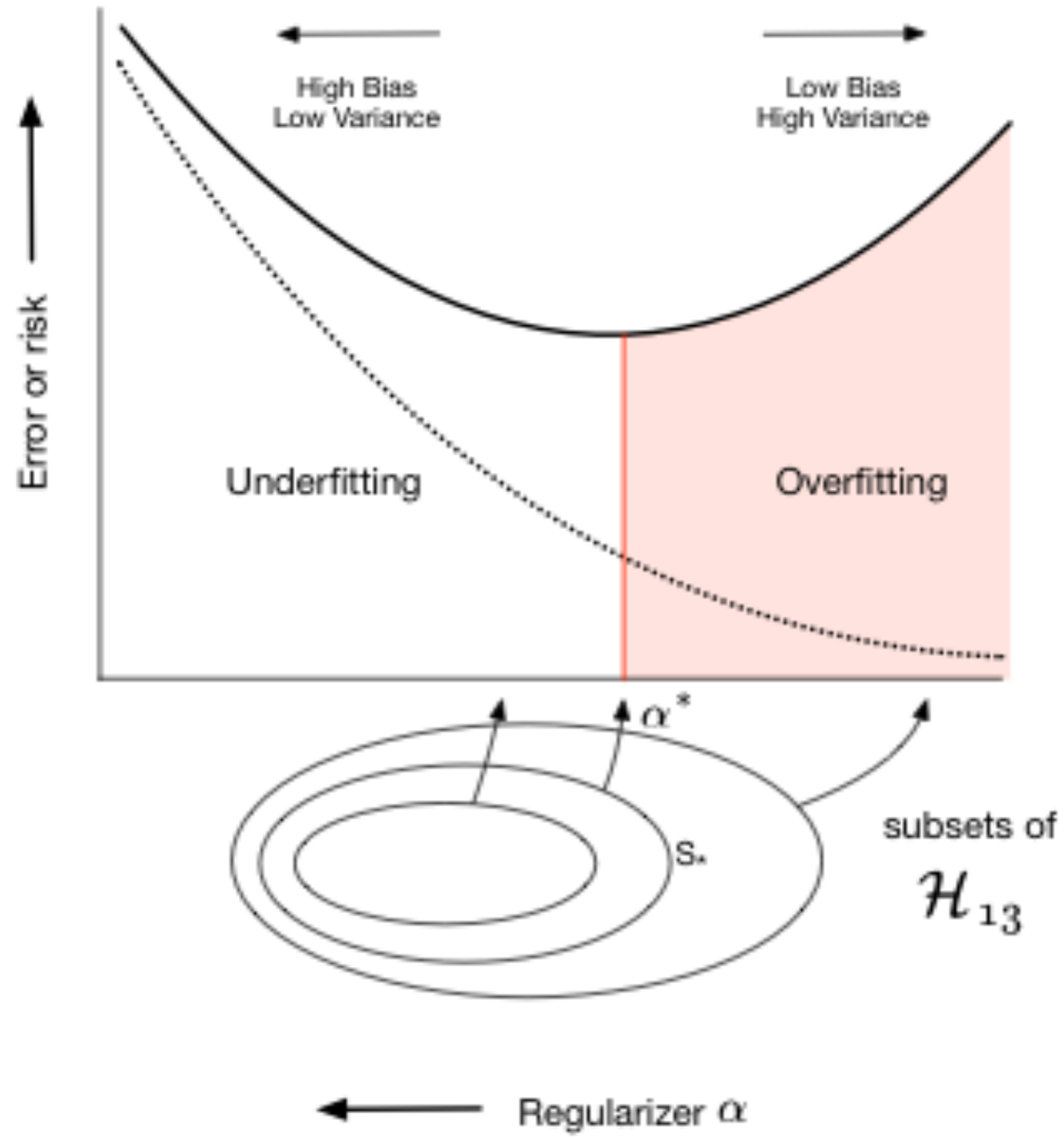
Keep higher a-priori complexity and impose a

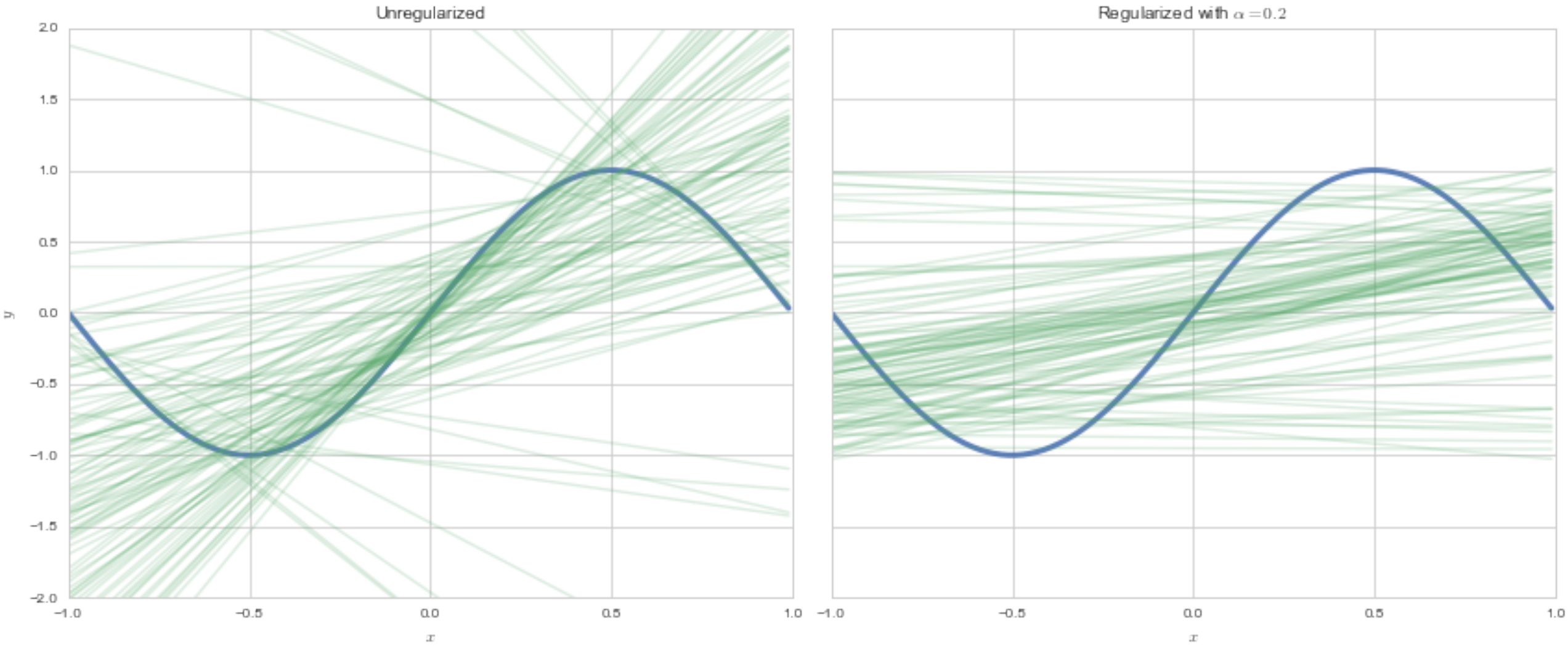
Restrict parameter values by regularization penalty

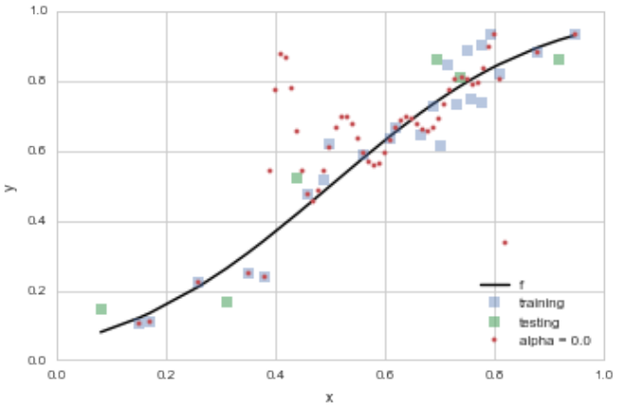
complexity penalty

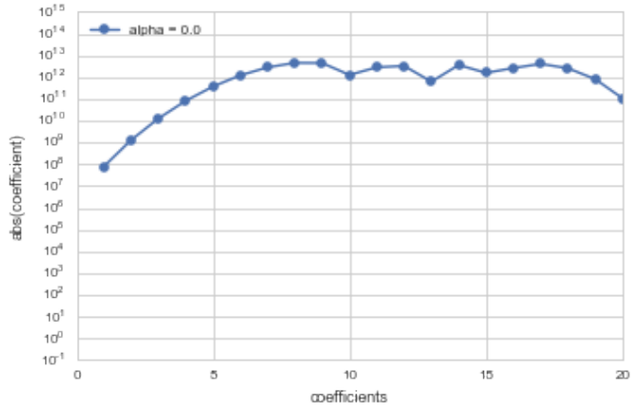
on risk instead, to choose a SUBSET of $\mathcal{H}_{big}$.
We'll make the coefficients small:

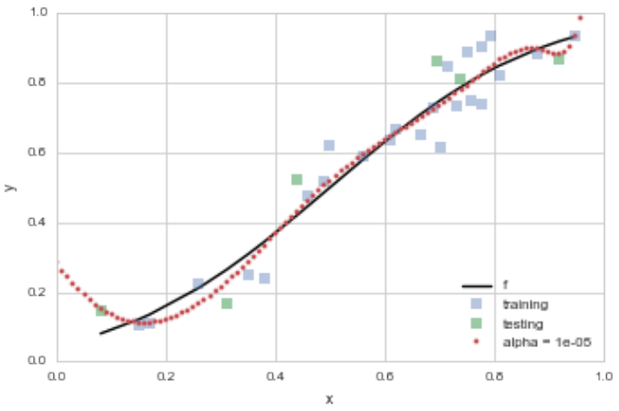
$$\sum_{i=0}^{j} \theta_i^2 < C.$$

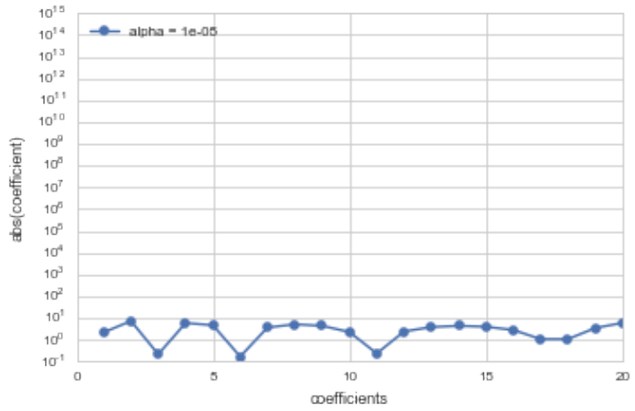


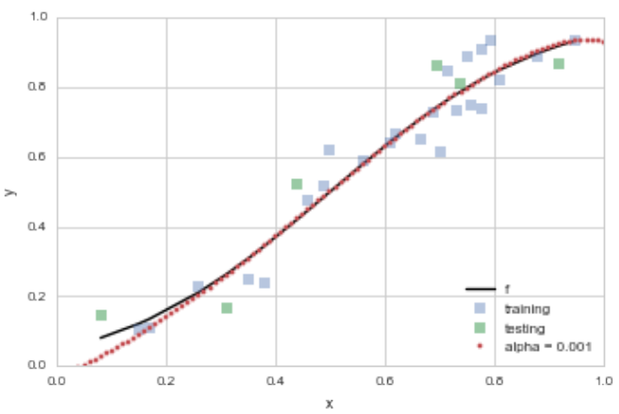

Unregularized
Regularized with $\alpha = 0.2$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
y
−1.0
−0.5
0.0
0.5
1.0
x

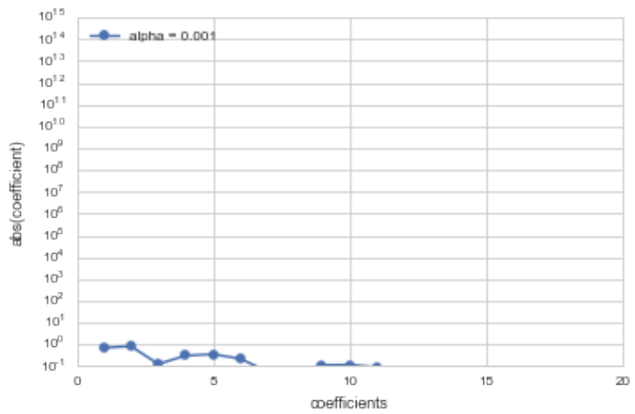


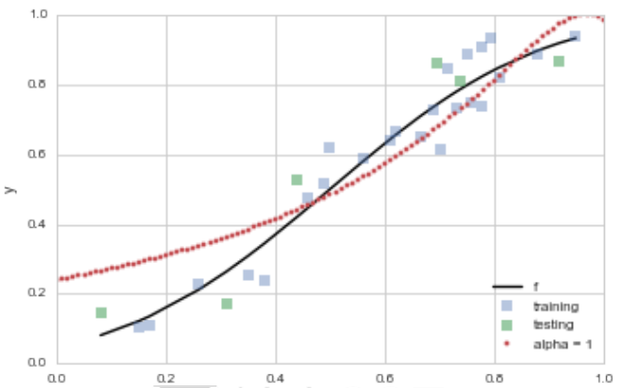


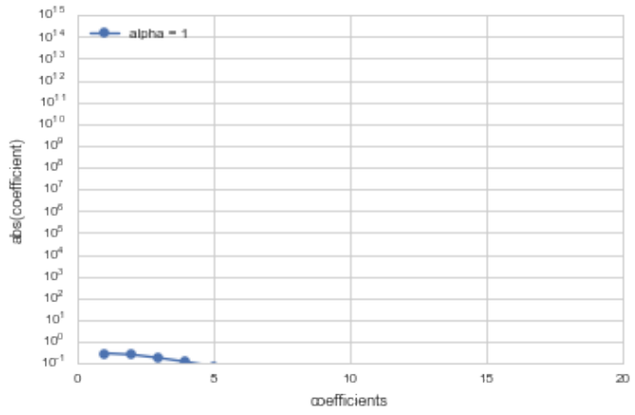












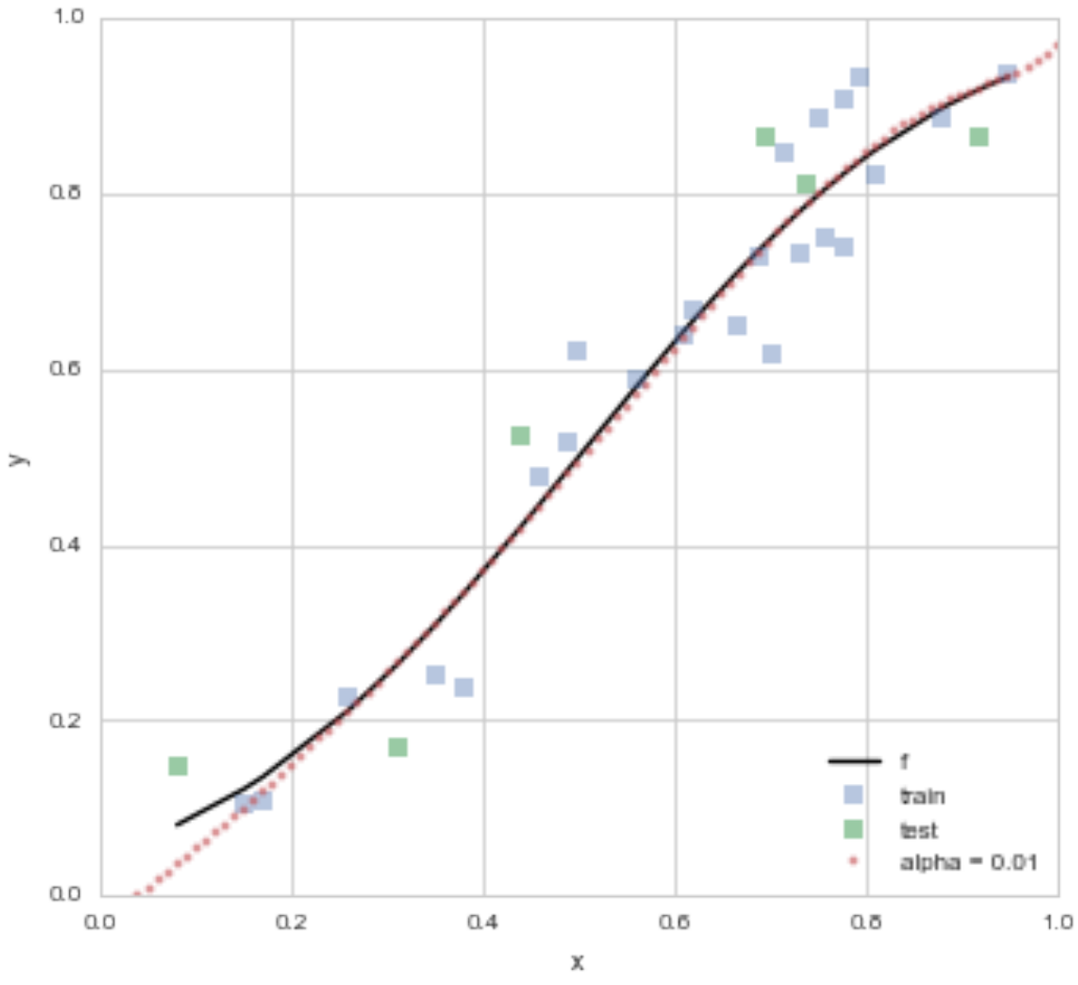
REGULARIZATION

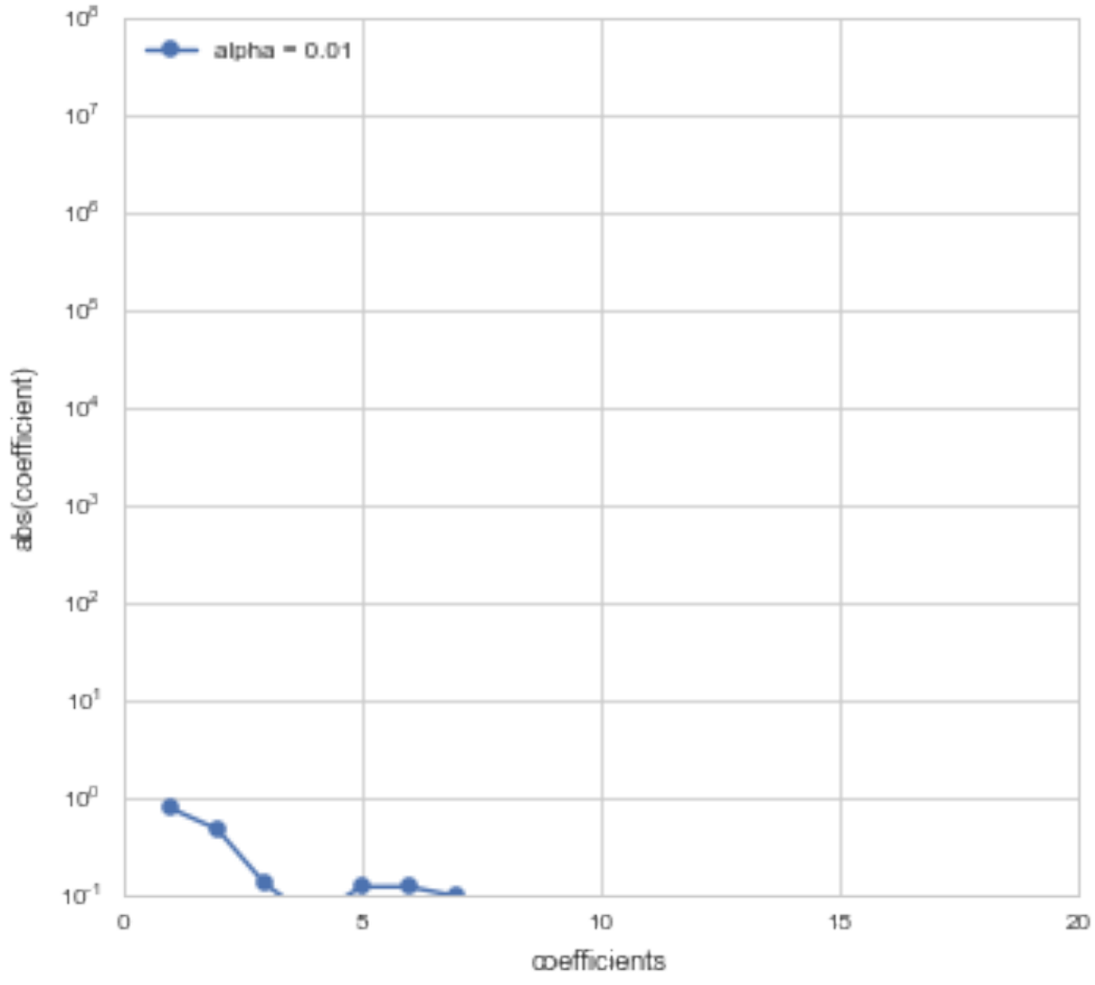
$$\mathcal{R}(h_j) = \sum_{y_i \in \mathcal{D}} (y_i - h_j(x_i))^2 + \alpha \sum_{i=0}^{j} \theta_i^2.$$

As we increase 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

1. having validation sets reduces the training data size
2. using validation sets also fits the model on the validation set, thus the model is more prone to overfit on the original data

- 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 $q(x)$.

KL divergence is always non-negative!

Divergence:

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

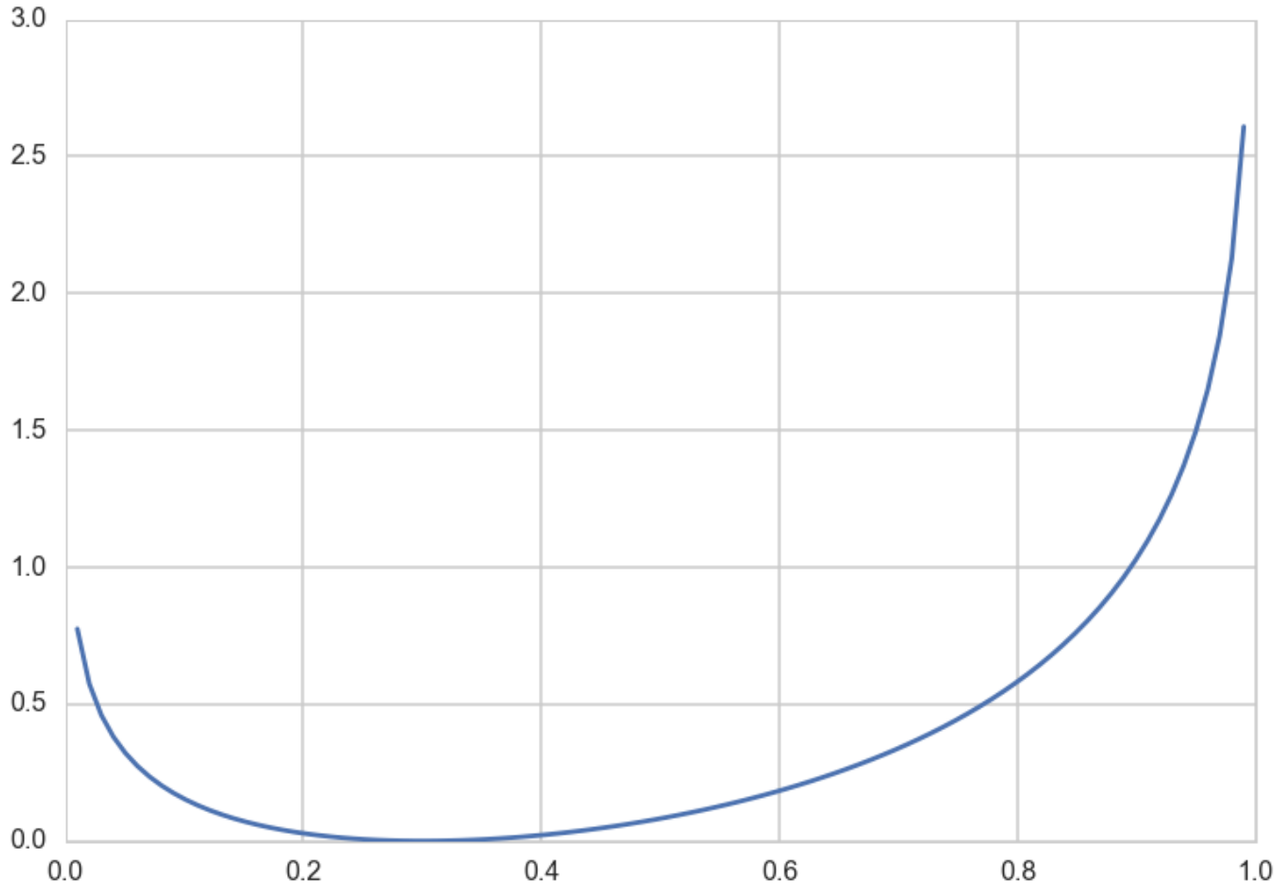
- McElreath page 179

KL example

Bernoulli Distribution p with $p = 0.3$.

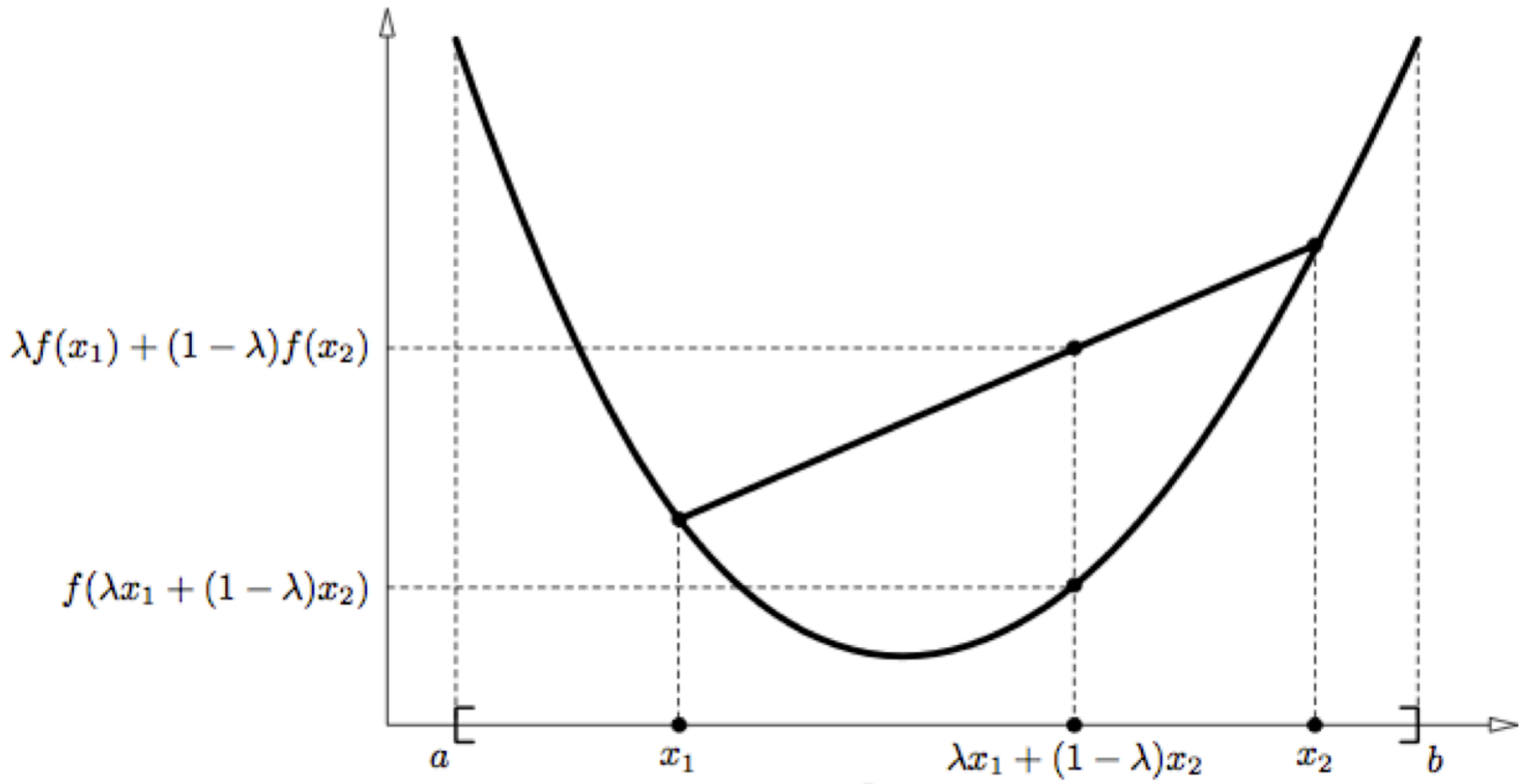
Try to approximate by q. What parameter?

```
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:

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

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

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

```
= -log(\int p* 1/p * q dq)
```

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 the observed data likelihood

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** ...

coeff = 2, coming from definition

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

Example

Generate data from:

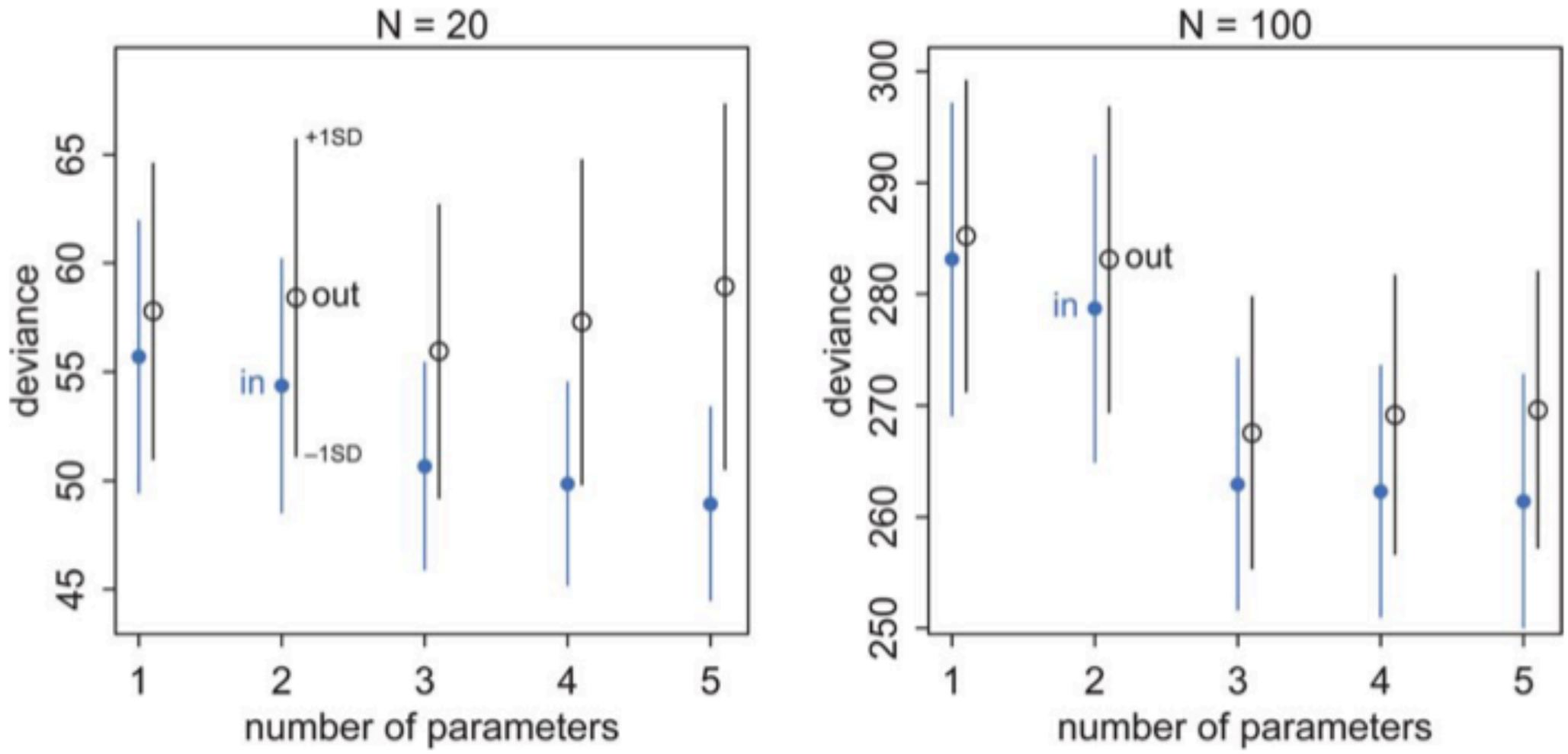
$$\mu_i = 0.15x_{1,i} - 0.4x_{2,i}\,,\;\; y \sim N(\mu, 1)$$

2 parameter model.

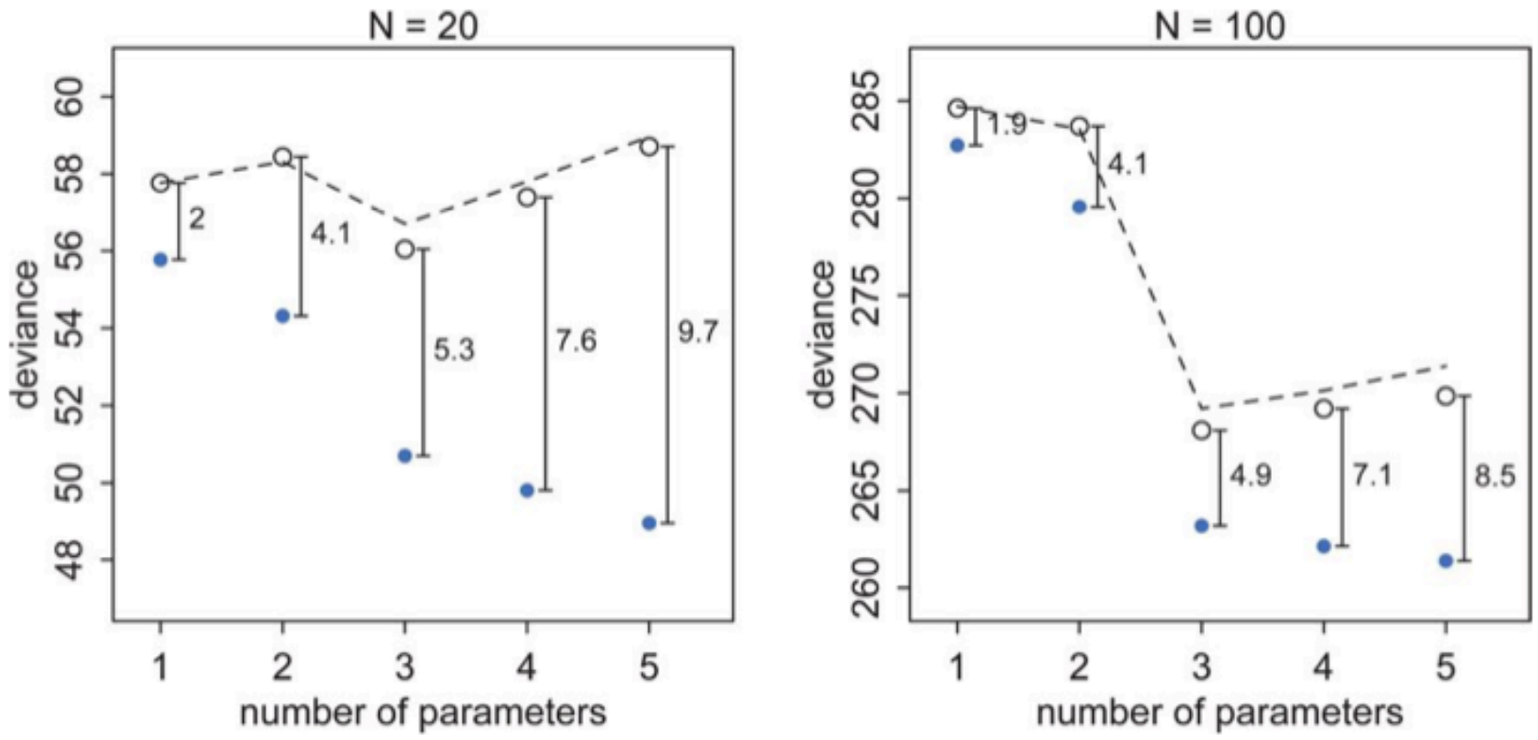
Generate 10,000 realizations, for 1-5 parameters, 20 data points and 100 data points.

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.

`p = number of parameters`

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

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

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

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

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

****Note**: AIC is dependent on the number of data points we have**

Information and Uncertainty

- coin at 50% odds has maximal uncertainty
- reflects my lack of knowledge of the physics
- many ways for 50% heads.

- an election with $p = 0.99$ has a lot of Information

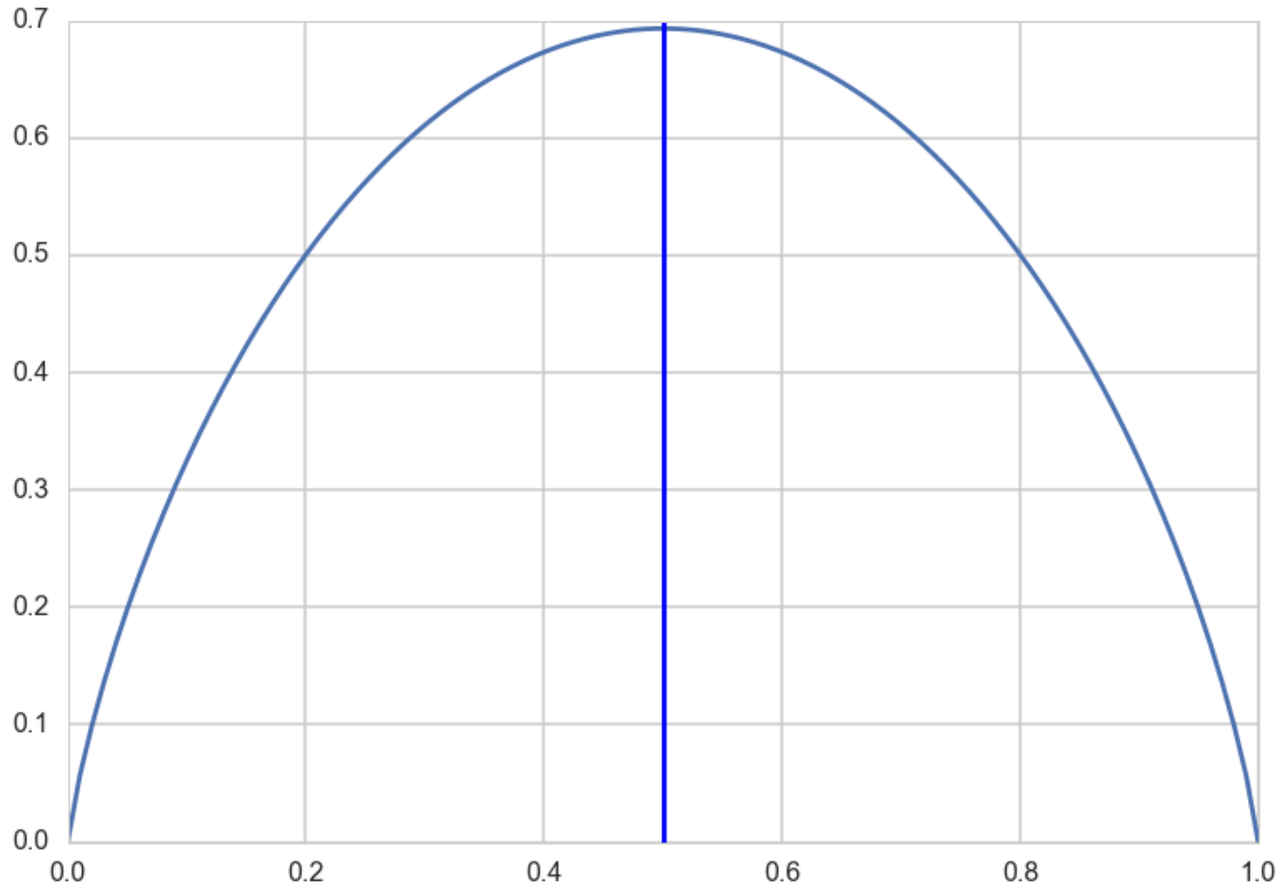
information is the reduction in uncertainty from learning an outcome

Information Entropy, a measure of uncertainty

Desiderata:
- must be continuous so that there are no jumps
- must be additive across events or states, and must increase as the number of events/states increases

$$H(p) = -E_p[log(p)] = -\int p(x)log(p(x))dx \;\; OR \; -\sum_i p_i log(p_i)$$

Entropy for coin fairness



$$H(p) = -E_p[log(p)] = -p * log(p) - (1-p) * log(1-p)$$

```
def h(p):
    if p==1.:
        ent = 0
    elif p==0.:
        ent = 0
    else:
        ent = - (p*math.log(p) + (1-p)* math.log(1-p))
```

Maximum Entropy (MAXENT)

- finding distributions consistent with constraints and the current state of our information
- what would be the least surprising distribution?
- The one with the least additional assumptions?

The distribution that can happen in the most ways is the one with the highest entropy

For a gaussian

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$

$$H(p) = E_p[log(p)] = E_p[-\frac{1}{2}log(2\pi\sigma^2) - (x-\mu)^2/2\sigma^2]$$

$$= -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2\sigma^2}E_p[(x-\mu)^2] = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2} = \frac{1}{2}log(2\pi e\sigma^2)$$

Cross Entropy

$$H(p, q) = -E_p[log(q)]$$

Then one can write:

$$D_{KL}(p, q) = H(p, q) - H(p)$$

KL-Divergence is additional entropy introduced by using q instead of p.

We saw this for Logistic regression

- $H(p, q)$ and $D_{KL}(p, q)$ are not symmetric.
- if you use a unusual , low entropy distribution to approximate a usual one, you will be more surprised than if you used a high entropy, many choices one to approximate an unusual one.

Corollary: if we use a high entropy distribution to approximate the true one, we will incur lesser error.

Gaussian is MAXENT for fixed mean and variance

Consider
$D_{KL}(q,p) = E_q[log(q/p)] = H(q,p) - H(q) >= 0$

$$H(q,p) = E_q[log(p)] = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2\sigma^2}E_q[(x-\mu)^2]$$

$E_q[(x-\mu)^2]$ is CONSTRAINED to be σ^2.

$$H(q,p) = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2} = -\frac{1}{2}log(2\pi e\sigma^2) = H(p) >= H(q)!!!$$

Importance of MAXENT

- most common distributions used as likelihoods (and priors) are in the exponential family, MAXENT subject to different constraints.
- gamma: MAXENT all distributions with the same mean and same average logarithm.
- exponential: MAXENT all non-negative continuous distributions with the same average inter-event displacement

Importance of MAXENT

- Information entropy enumerates the number of ways a distribution can arise, after having fixed some assumptions.
- choosing a maxent distribution as a likelihood means that once the constraints has been met, no additional assumptions.

The most conservative distribution

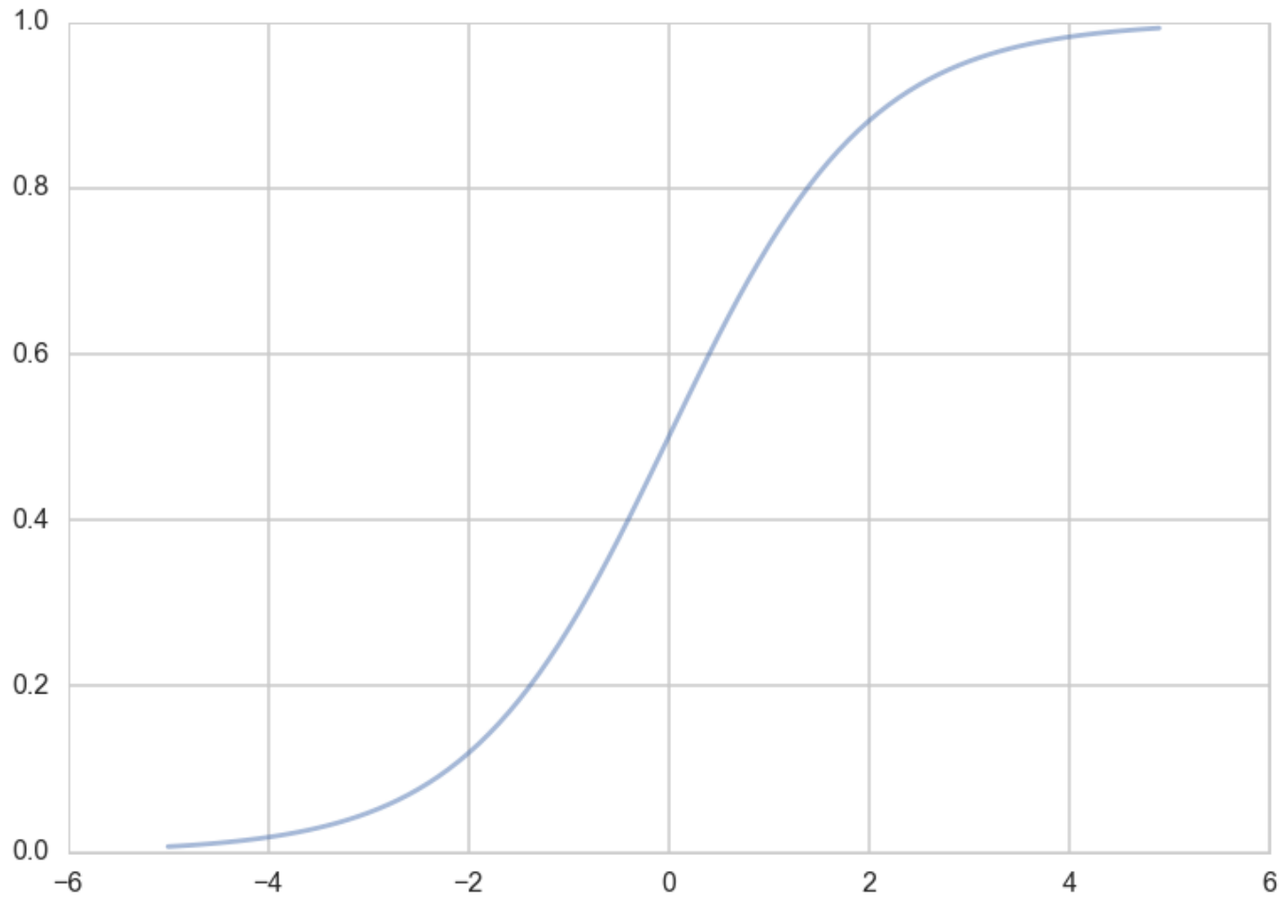
MLE for Logistic Regression

- example of a Generalized Linear Model (GLM)
- "Squeeze" linear regression through a **Sigmoid** function
- this bounds the output to be a probability
- What is the sampling Distribution?

Sigmoid function

This function is plotted below:

```
h = lambda z: 1./(1+np.exp(-z))
zs=np.arange(-5,5,0.1)
plt.plot(zs, h(zs), alpha=0.5);
```



Identify: $z = \mathbf{w} \cdot \mathbf{x}$ and $h(\mathbf{w} \cdot \mathbf{x})$ with the probability that the sample is a '1' ($y = 1$).

Then, the conditional probabilities of $y = 1$ or $y = 0$ given a particular sample's features $\mathbf{x}$ are:

$$P(y = 1|\mathbf{x}) = h(\mathbf{w} \cdot \mathbf{x})$$
$$P(y = 0|\mathbf{x}) = 1 - h(\mathbf{w} \cdot \mathbf{x}).$$

These two can be written together as

$$P(y|\mathbf{x}, \mathbf{w}) = h(\mathbf{w} \cdot \mathbf{x})^y (1 - h(\mathbf{w} \cdot \mathbf{x}))^{(1-y)}$$

BERNOULLI!!

Multiplying over the samples we get:

$$P(y|\mathbf{x},\mathbf{w}) = P(\{y_i\}|\{\mathbf{x}_i\},\mathbf{w}) = \prod_{y_i \in \mathcal{D}} P(y_i|\mathbf{x}_i,\mathbf{w}) = \prod_{y_i \in \mathcal{D}} h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i}\left(1-h(\mathbf{w}\cdot\mathbf{x}_i)\right)^{(1-y_i)}$$

A noisy y is to imagine that our data $\mathcal{D}$ was generated from a joint probability distribution $P(x, y)$. Thus we need to model y at a given x, written as $P(y \mid x)$, and since $P(x)$ is also a probability distribution, we have:

$$P(x, y) = P(y \mid x)P(x),$$

Indeed its important to realize that a particular sample can be thought of as a draw from some "true" probability distribution.

maximum likelihood estimation maximises the **likelihood of the sample y**,

$$\mathcal{L} = P(y \mid \mathbf{x}, \mathbf{w}).$$

Again, we can equivalently maximize

$$\ell = log(P(y \mid \mathbf{x}, \mathbf{w}))$$

Thus

$$\begin{aligned}
\ell &= log\left(\prod_{y_i \in \mathcal{D}} h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i} \left(1 - h(\mathbf{w}\cdot\mathbf{x}_i)\right)^{(1-y_i)}\right) \\
&= \sum_{y_i \in \mathcal{D}} log\left(h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i} \left(1 - h(\mathbf{w}\cdot\mathbf{x}_i)\right)^{(1-y_i)}\right) \\
&= \sum_{y_i \in \mathcal{D}} log\, h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i} + log\left(1 - h(\mathbf{w}\cdot\mathbf{x}_i)\right)^{(1-y_i)} \\
&= \sum_{y_i \in \mathcal{D}} (y_i log(h(\mathbf{w}\cdot\mathbf{x})) + (1-y_i) log(1 - h(\mathbf{w}\cdot\mathbf{x})))
\end{aligned}$$

Use Convex optimization! (soon, hw)