$\LaTeX$ command declarations here.

In [1]:
```
from __future__ import division

# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
import seaborn as sns
import pylab as pl
from matplotlib.pylab import cm
import pandas as pd


# scientific
import numpy as np;

# ipython
from IPython.display import Image
```

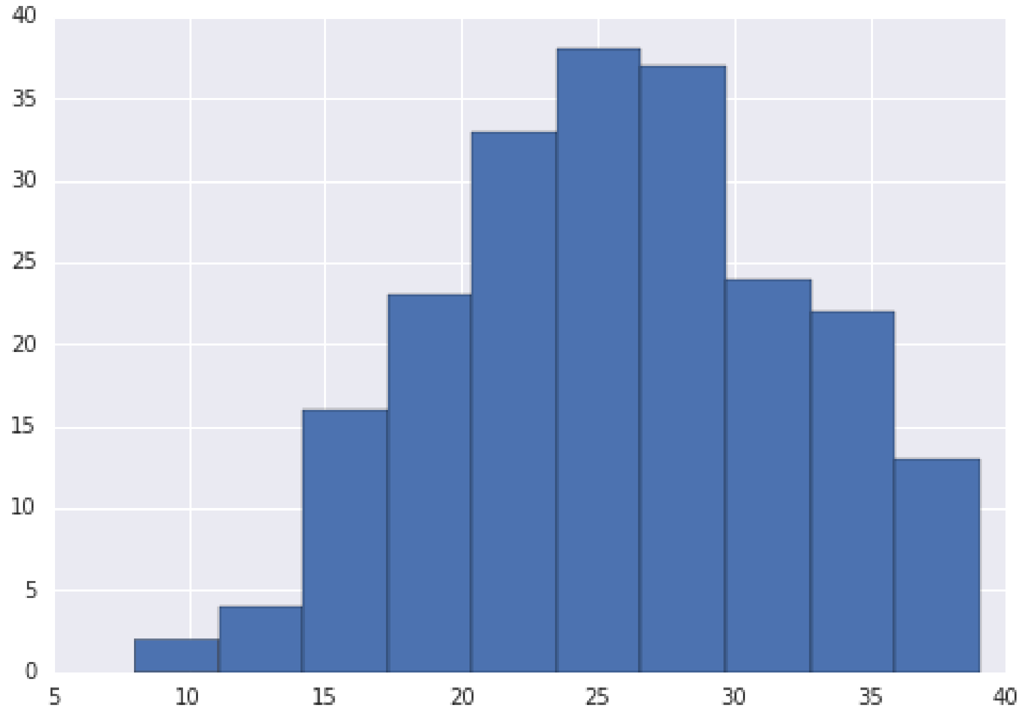
EECS 545: Machine Learning

Lecture 13: Information Theory and Exponential Families ¶

- Instructor: **Jacob Abernethy**
- Date: March 7, 2016

Lecture Exposition Credit: Benjamin Bray & Saket Dewangan

Midterm performance: Not Bad!



- Mean: 25.79, Median: 25.5, StdDev: 6.47

Optional Final Project

- Project is **very optional**. Students should only do project if they are serious and enthusiastic.
- Groups encouraged, up to 4 per group (effort should scale accordingly!)
- 1-page proposal due **March 23rd**, final project due **April 21**
- Projects can involve (a) new algorithms and experiments, (b) a new and exciting application, (c) literature survey, (d) a replication of published work.
- Do not submit projects from other courses! We can tell...

Optional Final Project Grading Policy

- Students submitting a project are subject to alternative grading scheme.

	Basic Scheme	With Project
Midterm	25%	18%
Final Exam	25%	18%
Project	0%	18%

- Project can help your grade, but it **can also hurt**!
- Students must commit to Project grading, but can withdraw up to April 11th.

Review of Bias-Variance Tradeoff

Bias and Variance Formulae

- Recall $y = f + \epsilon$, where ϵ is some 0-mean noise with var. σ^2
- Alg receives dataset S and outputs $\hat{f}$, prediction of y. The error is:

$$\mathbb{E}[(y - \hat{f})^2] = \underbrace{\sigma^2}_{\text{irreducible error}} + \underbrace{\mathrm{Var}[\hat{f}]}_{\text{Variance}} + \underbrace{\mathbb{E}[f - \mathbb{E}_S[\hat{f}]]^2}_{\text{Bias}^2}$$

- Break error into two terms relating to $\mathbb{E}_S[\hat{f}]$ the "average" estimate over random datasets S.
  - Bias of an estim.: $\mathrm{Bias}(\hat{f}) = (\mathbb{E}_S[\hat{f}] - f)$
  - Variance of estim.: $\mathrm{Var}(\hat{f}) = \mathbb{E}[(\hat{f} - \mathbb{E}_S[\hat{f}])^2]$

An example to explain Bias/Variance and illustrate the tradeoff

- Consider estimating a sinusoidal function.

(Example that follows is inspired by Yaser Abu-Mostafa's CS 156 Lecture titled "Bias-Variance Tradeoff"

In [2]:
```
RANGEXS = np.linspace(0., 2., 300)
TRUEYS = np.sin(np.pi * RANGEXS)

def plot_fit(x, y, p, show,color='k'):
    xfit = RANGEXS
    yfit = np.polyval(p, xfit)
    if show:
        axes = pl.gca()
        axes.set_xlim([min(RANGEXS),max(RANGEXS)])
        axes.set_ylim([-2.5,2.5])
        pl.scatter(x, y, facecolors='none', edgecolors=color)
        pl.plot(xfit, yfit,color=color)
        pl.hold('on')
        pl.xlabel('x')
        pl.ylabel('y')
```

In [3]:
```
def calc_errors(p):
    x = RANGEXS
    errs = []
    for i in x:
        errs.append(abs(np.polyval(p, i) - np.sin(np.pi * i)) **
2)
    return errs
```

In [4]:
```
def calculate_bias_variance(poly_coeffs, input_values_x, true_va
lues_y):
    # poly_coeffs: a list of polynomial coefficient vectors
    # input_values_x: the range of xvals we will see
    # true_values_y: the true labels/targes for y

    # First we calculate the mean polynomial, and compute the pr
edictions for this mean poly
    mean_coeffs = np.mean(poly_coeffs, axis=0)
    mean_predicted_poly = np.poly1d(mean_coeffs)
    mean_predictions_y = np.polyval(mean_predicted_poly, input_v
alues_x)

    # Then we calculate the error of this mean poly
    bias_errors_across_x = (mean_predictions_y - true_values_y)
** 2

    # To consider the variance errors, we need to look at every
output of the coefficients
    variance_errors = []
    for coeff in poly_coeffs:
        predicted_poly = np.poly1d(coeff)
        predictions_y = np.polyval(predicted_poly, input_values_
x)
        # Variance error is the average squared error between th
e predicted values of y
        # and the *average* predicted value of y
        variance_error = (mean_predictions_y - predictions_y)**2
        variance_errors.append(variance_error)

    variance_errors_across_x = np.mean(np.array(variance_error
s),axis=0)

    return bias_errors_across_x, variance_errors_across_x
```

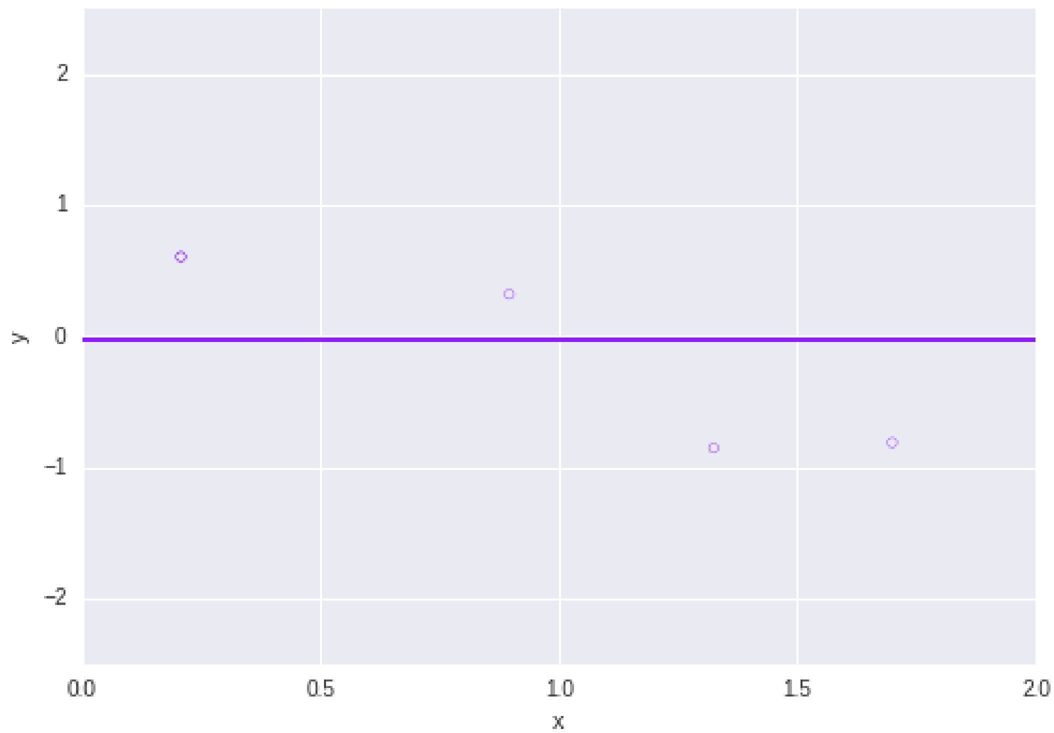
In [5]:
```
def polyfit_sin(degree=0, iterations=100, num_points=5, show=True):
    total = 0
    l = []
    coeffs = []
    errs = [0] * len(RANGEXS)
    colors=cm.rainbow(np.linspace(0,1,iterations))
    for i in range(iterations):
        np.random.seed()
        x = np.random.choice(RANGEXS,size=num_points) # Pick random points from the sinusoid
        y = np.sin(np.pi * x)
        p = np.polyfit(x, y, degree)
        y_poly = [np.polyval(p, x_i) for x_i in x]
        plot_fit(x, y, p, show,color=colors[i])
        total += sum(abs(y_poly - y) ** 2) # calculate Squared Error (Squared Error)
        coeffs.append(p)
        errs = np.add(calc_errors(p), errs)
    return total / iterations, errs / iterations, np.mean(coeffs, axis = 0), coeffs
```

In [6]:
```
def plot_bias_and_variance(biases,variances,range_xs,true_ys,mean_predicted_ys):
    pl.plot(range_xs, mean_predicted_ys, c='k')
    axes = pl.gca()
    axes.set_xlim([min(range_xs),max(range_xs)])
    axes.set_ylim([-3,3])
    pl.hold('on')
    pl.plot(range_xs, true_ys,c='b')
    pl.errorbar(range_xs, mean_predicted_ys, yerr = biases, c='y', ls="None", zorder=0,alpha=1)
    pl.errorbar(range_xs, mean_predicted_ys, yerr = variances, c='r', ls="None", zorder=0,alpha=0.1)
    pl.xlabel('x')
    pl.ylabel('y')
```

Let's return to fitting polynomials

- Here we generate some samples x, y, with $y = \sin(2\pi x)$
- We then fit a degree-0 polynomial (i.e. a constant function) to the samples

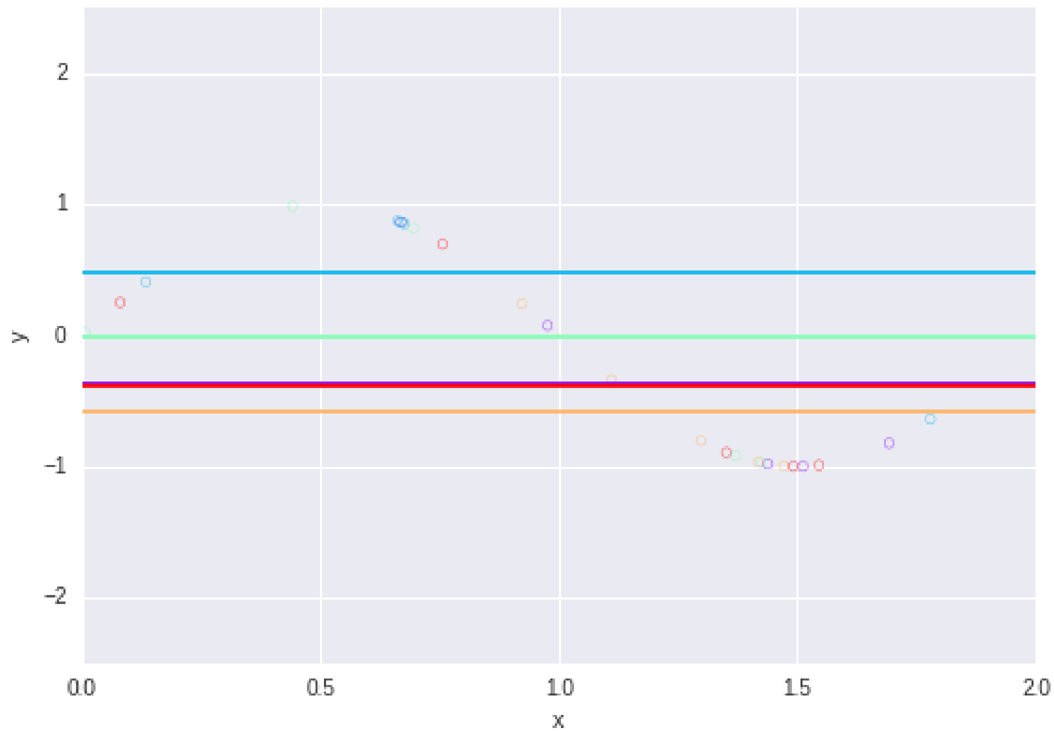
In [7]:
```
# polyfit_sin() generates 5 samples of the form (x,y) where y=si
n(2*pi*x)
# then it tries to fit a degree=0 polynomial (i.e. a constant fu
nc.) to the data
# Ignore return values for now, we will return to these later
_, _, _, _ = polyfit_sin(degree=0, iterations=1, num_points=5, s
how=True)
```



We can do this over many datasets

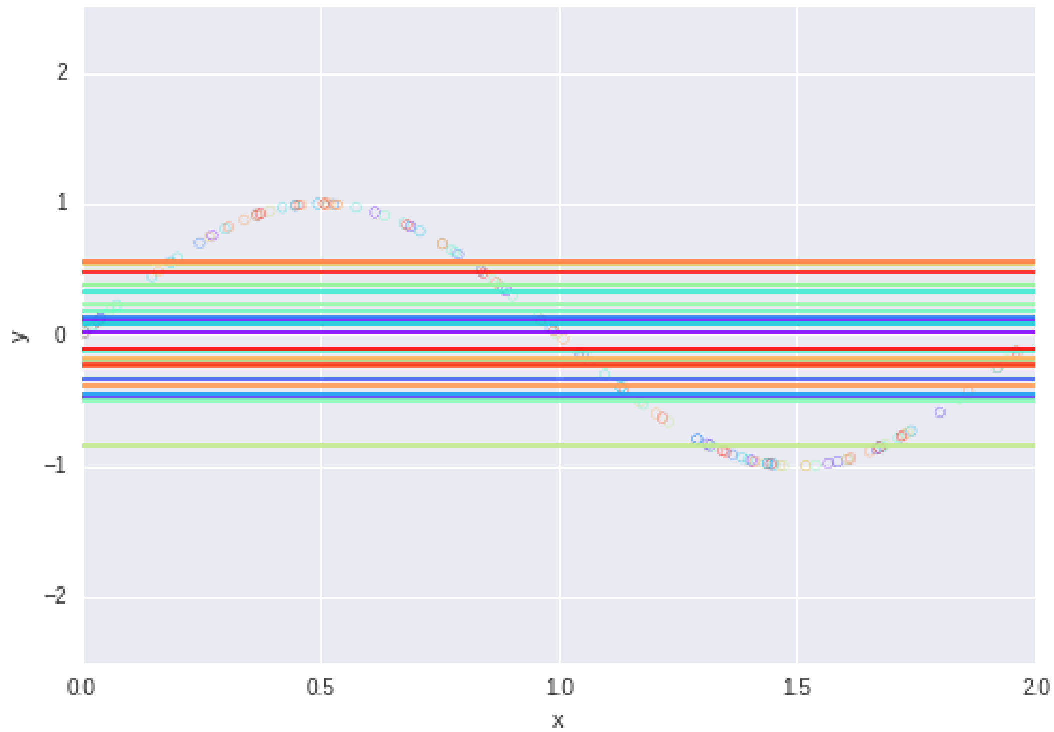
- Let's sample a number of datasets
- How does the fitted polynomial change for different datasets?

In [8]:
```
# Estimate two points of sin(pi * x) with a constant 5 times
_, _, _, _ = polyfit_sin(0, 5)
```

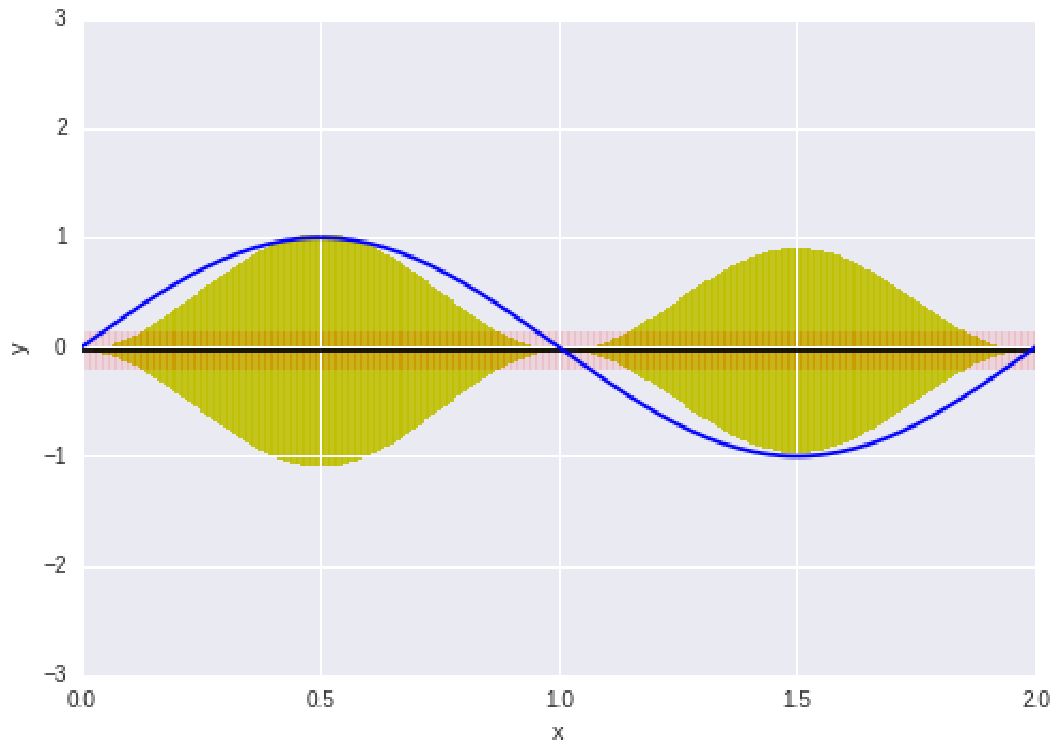


What about over lots more datasets?

In [9]:
```
# Estimate two points of sin(pi * x) with a constant 100 times
_, _, _, _ = polyfit_sin(0, 25)
```



In [10]:
```
MSE, errs, mean_coeffs, coeffs_list = polyfit_sin(0, 100,num_poi
nts = 3,show=False)
biases, variances = calculate_bias_variance(coeffs_list,RANGEXS,
TRUEYS)
plot_bias_and_variance(biases,variances,RANGEXS,TRUEYS,np.polyva
l(np.poly1d(mean_coeffs), RANGEXS))
```



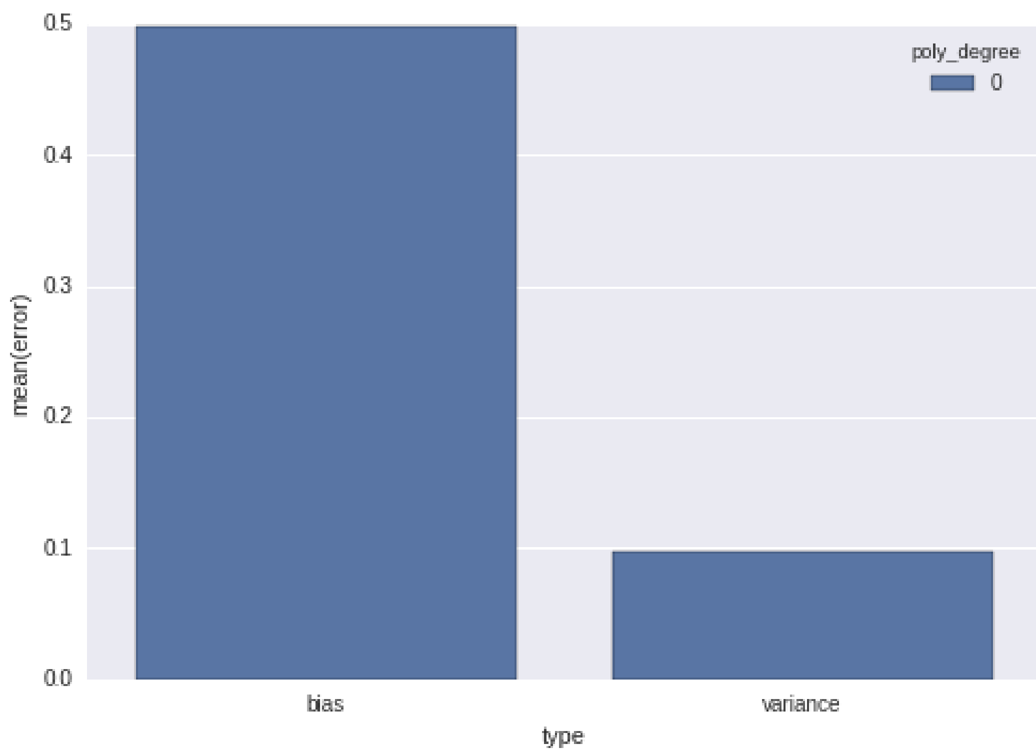
- Decomposition: $\mathbb{E}[(y - \hat{f})^2] = \underbrace{\sigma^2}_{\text{irreducible error}} + \underbrace{\mathrm{Var}[\hat{f}]}_{\text{Variance}} + \underbrace{\mathbb{E}[f - \mathbb{E}_S[\hat{f}]]^2}_{\text{Bias}^2}$
- Blue curve: true f
- Black curve: $\hat{f}$, average predicted values of y
- Yellow is error due to **Bias**, Red/Pink is error due to **Variance**

Bias vs. Variance

- We can calculate how much error we suffered due to bias and due to variance

In [11]:
```
poly_degree = 0
results_list = []
MSE, errs, mean_coeffs, coeffs_list = polyfit_sin(
    poly_degree, 500,num_points = 5,show=False)
biases, variances = calculate_bias_variance(coeffs_list,RANGEXS,
TRUEYS)
sns.barplot(x='type', y='error',hue='poly_degree', data=pd.DataF
rame([
    {'error':np.mean(biases), 'type':'bias','poly_degree':0},
    {'error':np.mean(variances), 'type':'variance','poly_degre
e':0}]))
```

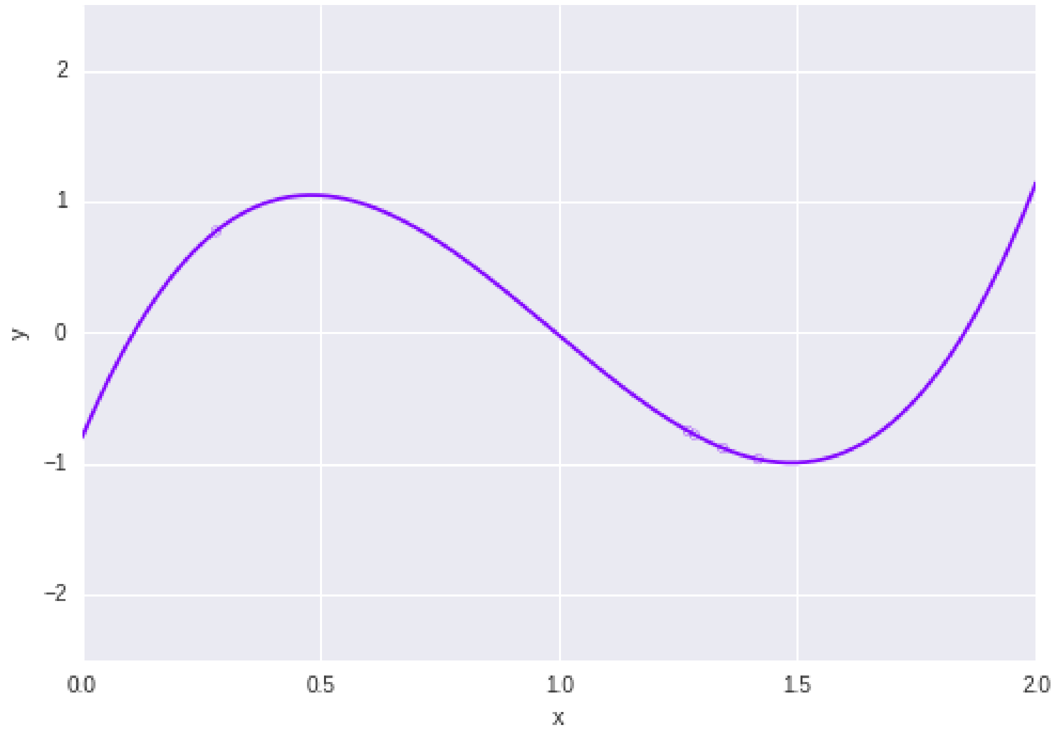
Out[11]: <matplotlib.axes._subplots.AxesSubplot at 0x7fd59974b828>



Let's now fit degree=3 polynomials

- Let's sample a dataset of 5 points and fit a cubic poly

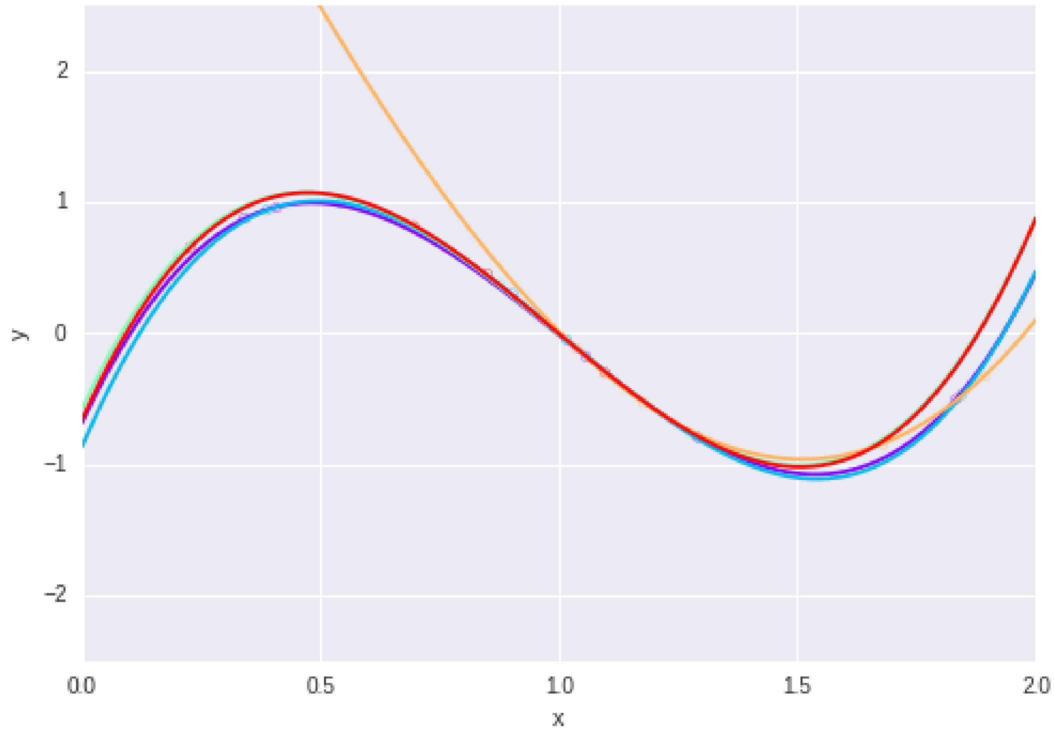
In [12]:
```
MSE, _, _, _ = polyfit_sin(degree=3, iterations=1)
```



Let's now fit degree=3 polynomials

- What does this look like over 5 different datasets?

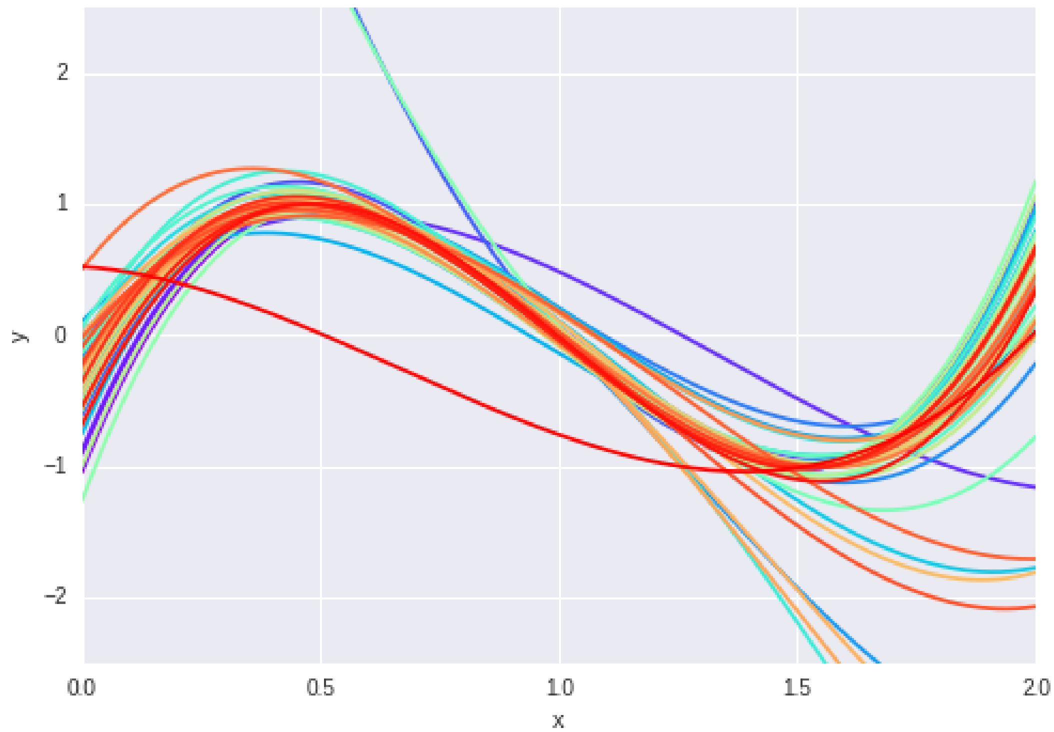
In [13]:
```
_, _, _, _ = polyfit_sin(degree=3,iterations=5,num_points=5,show=True)
```



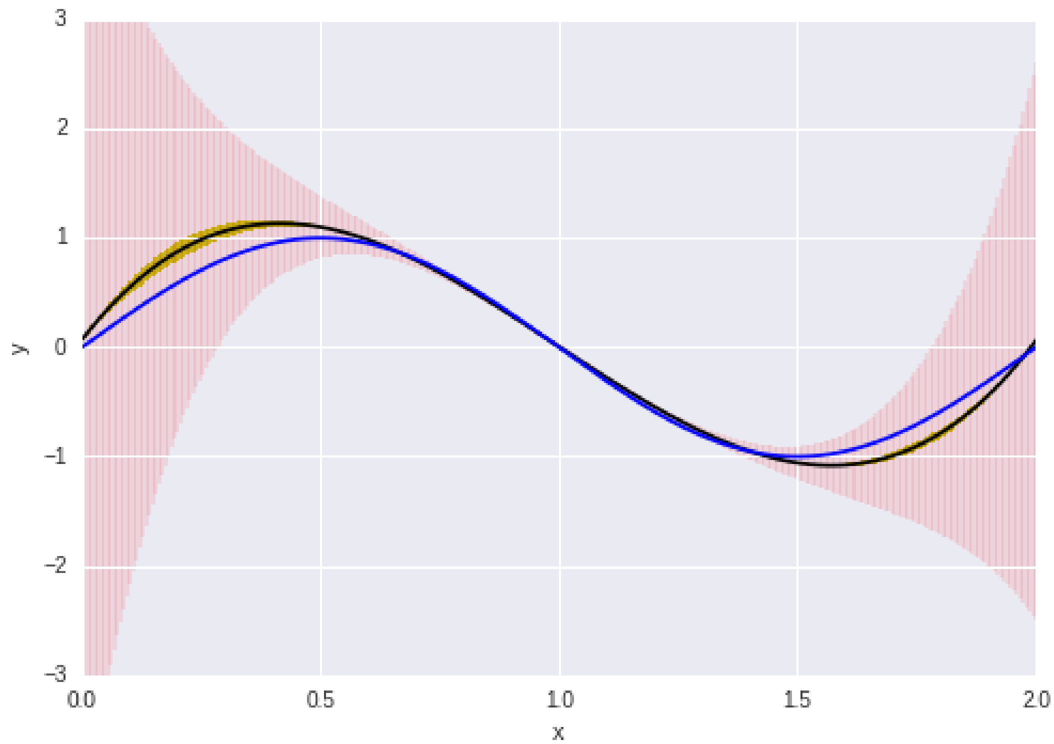
Let's now fit degree=3 polynomials

- What does this look like over 50 different datasets?

In [14]:
```
# Estimate two points of sin(pi * x) with a line 50 times
_, _, _, _ = polyfit_sin(degree=3, iterations=50)
```



In [15]:
```
MSE, errs, mean_coeffs, coeffs_list = polyfit_sin(3,500,show=False)
biases, variances = calculate_bias_variance(coeffs_list,RANGEXS,TRUEYS)
plot_bias_and_variance(biases,variances,RANGEXS,TRUEYS,np.polyval(np.poly1d(mean_coeffs), RANGEXS))
```



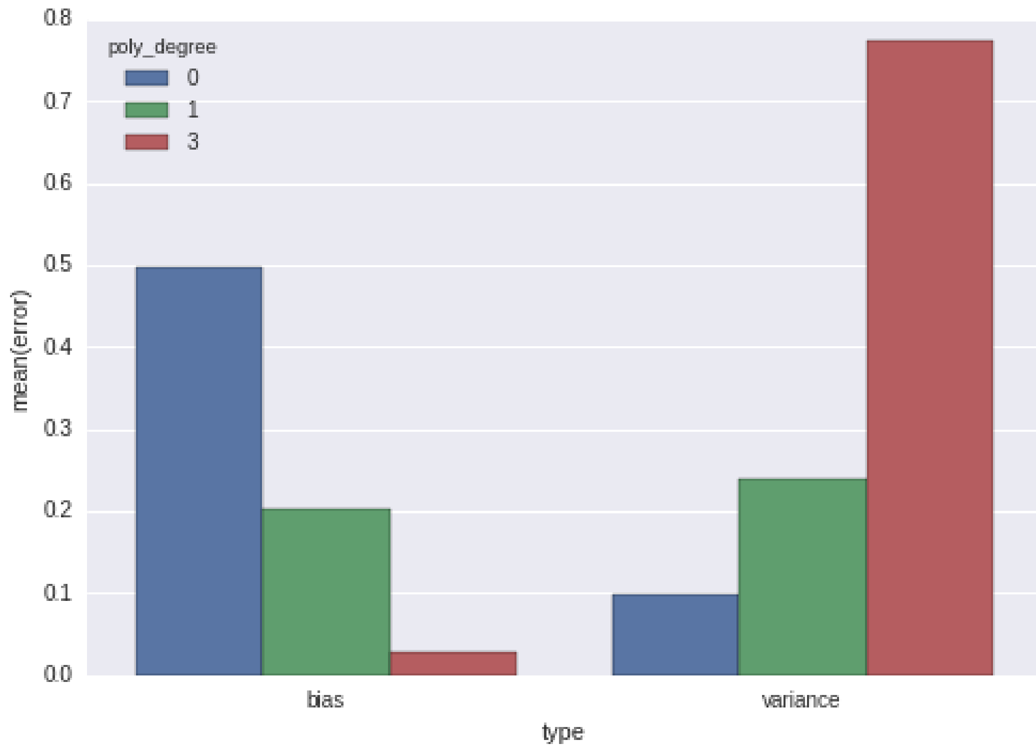
$$\mathbb{E}[(y-\hat{f})^2] = \underbrace{\sigma^2}_{\text{irreducible error}} + \underbrace{\mathrm{Var}[\hat{f}]}_{\text{Variance}} + \underbrace{\mathbb{E}[f-\mathbb{E}_S[\hat{f}]]^2}_{\text{Bias}^2}$$

- Blue curve: true f
- Black curve: $\mathbb{E}[\hat{f}]$, average prediction of y
- Yellow is error due to **Bias**, Red/Pink is error due to **Variance**

Bias and Variance for different degree sizes

In [16]:
```
results_list = []
for poly_degree in [0,1,3]:
    MSE, errs, mean_coeffs, coeffs_list = polyfit_sin(poly_degree,500,num_points=5,show=False)
    biases, variances = calculate_bias_variance(coeffs_list,RANGEXS,TRUEYS)
    results_list.append({'error':np.mean(biases),
                         'type':'bias', 'poly_degree':poly_degree})
    results_list.append({'error':np.mean(variances),
                         'type':'variance', 'poly_degree':poly_degree})
sns.barplot(x='type', y='error',hue='poly_degree',data=pd.DataFrame(results_list))
```

Out[16]: <matplotlib.axes._subplots.AxesSubplot at 0x7fd5985ef358>



- High degree polys have lower bias but much greater variance!

Info Theory + Exponential Familes -- References

Information Theory:

- **[Shannon 1951]** Shannon, Claude E.. *The Mathematical Theory of Communication* (http://worrydream.com/refs/Shannon%20-%20A%20Mathematical%20Theory%20of%20Communication.pdf). 1951.
- **[Pierce 1980]** Pierce, John R.. *An Introduction to Information Theory: Symbols, Signals, and Noise* (http://www.amazon.com/An-Introduction-Information-Theory-Mathematics/dp/0486240614). 1980.
- **[Stone 2015]** Stone, James V.. *Information Theory: A Tutorial Introduction* (http://jim-stone.staff.shef.ac.uk/BookInfoTheory/InfoTheoryBookMain.html). 2015.

Exponential Families:

- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[Hero 2008]** Hero, Alfred O.. *Statistical Methods for Signal Processing* (http://web.eecs.umich.edu/~hero/Preprints/main_564_08_new.pdf). 2008.
- **[Blei 2011]** Blei, David. *Notes on Exponential Families* (https://www.cs.princeton.edu/courses/archive/fall11/cos597C/lectures/exponential-families.pdf). 2011.
- **[Wainwright & Jordan 2008]** Wainwright, Martin J. and Michael I. Jordan. *Graphical Models, Exponential Families, and Variational Inference* (https://www.eecs.berkeley.edu/~wainwrig/Papers/WaiJor08_FTML.pdf). 2008.

Outline

This lecture, we introduce some important background for **Probabilistic Graphical Models**.

- Information Theory
  - Information, Entropy, and Encoding
  - Relative Entropy, Mutual Information & Collocations
  - Maximum Entropy Distributions
- Exponential Family
  - Mean and Natural Parameterizations
  - Conjugate Priors & Maximum Likelihood

Information Theory

> Uses material from **[MLAPP]** §2.8, **[Pierce 1980]**, **[Stone 2015]**, and **[Shannon 1951]**.

Information Theory

Information theory is concerned with

- **Compression:** Representing data in a compact fashion
- **Error Correction:** Transmitting and storing data in a way that is robust to errors

In machine learning, information-theoretic quantities are useful for

- manipulating probability distributions
- interpreting statistical learning algorithms

What is Information?

Can we measure the amount of **information** we gain from an observation?

- Information is measured in *bits* (don't confuse with *binary digits*, $0110001\ldots$)
- Intuitively, observing a fair coin flip should give 1 bit of information
- Observing two fair coins should give 2 bits, and so on...

Information: Definition

The **information content** of an event E with probability p is

$$I(E) = I(p) = -\log_2 p = \log_2 \frac{1}{p} \geq 0$$

- Information theory is about *probabilities* and *distributions*
- The "meaning" of events doesn't matter.
- Using bases other than 2 yields different units (Hartleys, nats, ...)

Example: Fair Coin

One Coin: If $P(Heads) = 0.5$ and we observe heads, then

$$I(Heads) = -\log_2 P(Heads) = 1 \text{ bit}$$

Two Coins: If we observe two heads in a row,

$$\begin{aligned} I(Heads, Heads) &= -\log_2 P(Heads, Heads) \\ &= -\log_2 P(Heads)P(Heads) \\ &= -\log_2 P(Heads) - \log_2 P(Heads) = 2 \text{ bits} \end{aligned}$$

Example: Unfair Coin

Suppose the coin has two heads, so $P(H) = 1$. Then,

$$I(Heads) = -\log_2 1 = 0$$

If we know the coin is unfair, we gain no information by observing heads!

- Information is a measure of how **surprised** we are by an outcome.
- Observing heads when $P(H) = 0$ yields *infinite* information.

Entropy: Definition

The **entropy** of a discrete random variable X with distribution p is

$$H[X] = H[p] = E[I(p(X))] = -\sum_{x \in X} p(x) \log p(x)$$

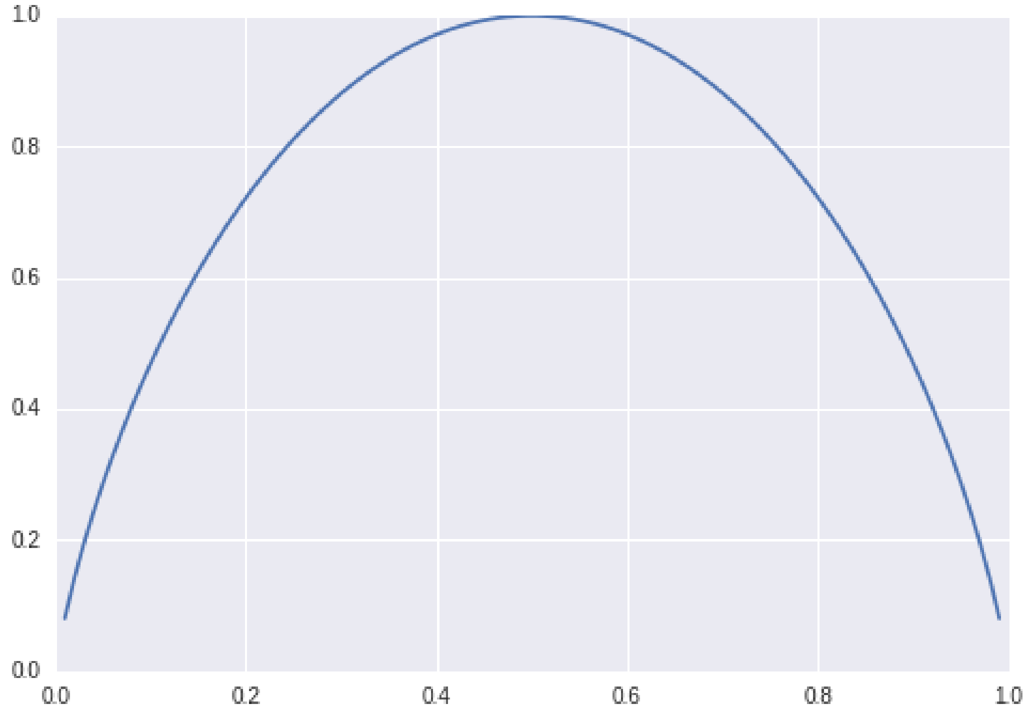
Entropy is the expected information received when we sample from X.

- How *surprised* are we, on average?

Entropy: Coin Flip

If X is binary, $H[X] = -[p \log p + (1-p) \log(1-p)]$

In [17]:
```
p = np.linspace(0.01,0.99,100);
plt.plot(p, -(p * np.log(p) + (1-p)*np.log(1-p)) / np.log(2));
```



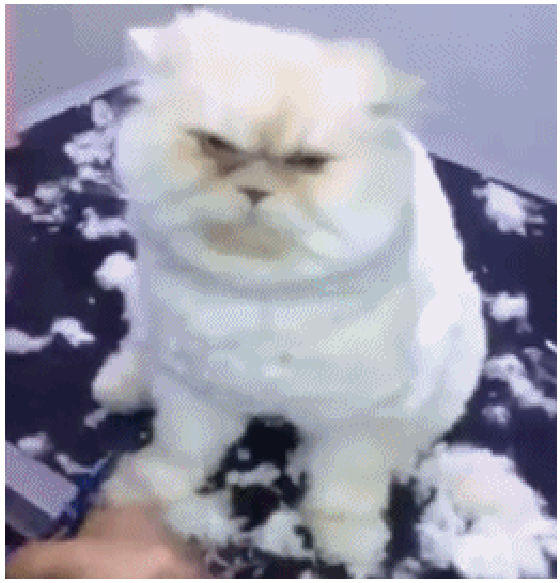
Entropy & Surprisal

Entropy is highest when X is close to uniform.

- Large entropy $\iff$ high uncertainty, more information from each new observation
- Low entropy $\iff$ more knowledge about possible outcomes

The farther from uniform X is, the lower the entropy.

Break Time!



Maximum Entropy Principle

Suppose we sample data from an unknown distribution p, and

- we collect statistics (mean, variance, etc.) from the data
- we want an *objective* or unbiased estimate of p

The **Maximum Entropy Principle** states that:

> We should choose p to have maximum entropy $H[p]$ among all distributions satisfying our constraints.

Maximum Entropy: Examples

Some examples of maximum entropy distributions:

Constraints	Maximum Entropy Distribution
Min a, Max b	Uniform $U[a, b]$
Mean μ, Support $(0, +\infty)$	Exponential $Exp(\mu)$
Mean μ, Variance σ^2	Gaussian $\mathcal{N}(\mu, \sigma^2)$

Later, **Exponential Family Distributions** will generalize this concept.

Communication Channels

For some intuition, consider a **communication channel**:

1. The **source** generates messages.
2. An **encoder** converts the message to a **signal** for transmission.
3. Signals are transmitted along a **channel**, possibly under the influence of **noise**.
4. A **decoder** attempts to reconstruct the original message from the transmitted signal.
5. The **destination** is the intended recipient.

In [18]:
```
Image(filename="images/shannon_comm_channel.jpg")
```

Out[18]:

34 The Mathematical Theory of Communication

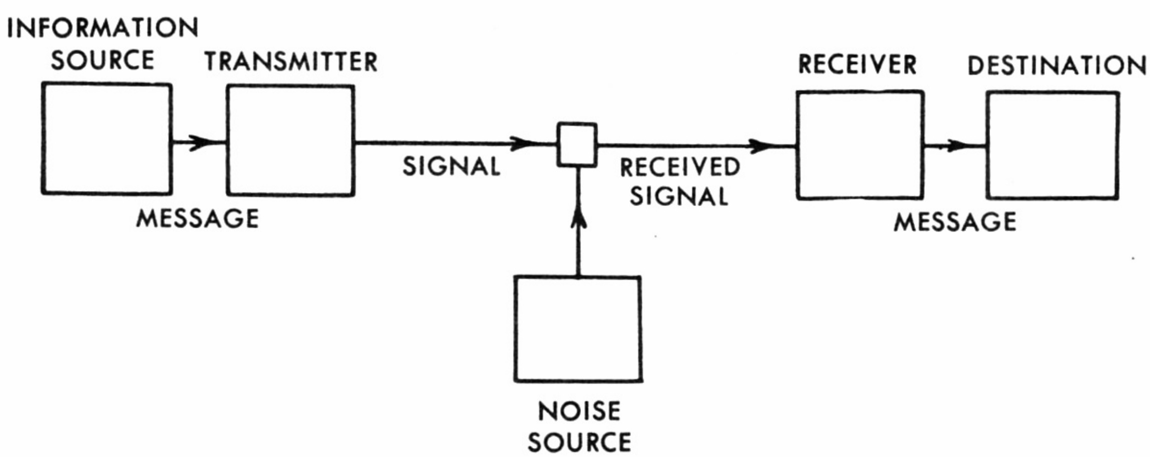


Fig. 1. — Schematic diagram of a general communication system.

Encoding

Suppose we draw messages from a distribution p.

- Certain messages may be more likely than others.
- For example, the letter e is most frequent in English

An **efficient** encoding minimizes the average message length,

- assign *short* codewords to common messages
- and *longer* codewords to rare messages

Interesting side note on Morse Code

At the time, newspaper printers had tiny metal copies of each letter, used for printing. A researcher apparently reasoned that they would have only as many copies of each letter as necessary to print a page, so he counted the number of copies of each letter they had and used that to estimate English letter frequencies.

Wikipedia reference (https://en.wikipedia.org/wiki/Morse_code)

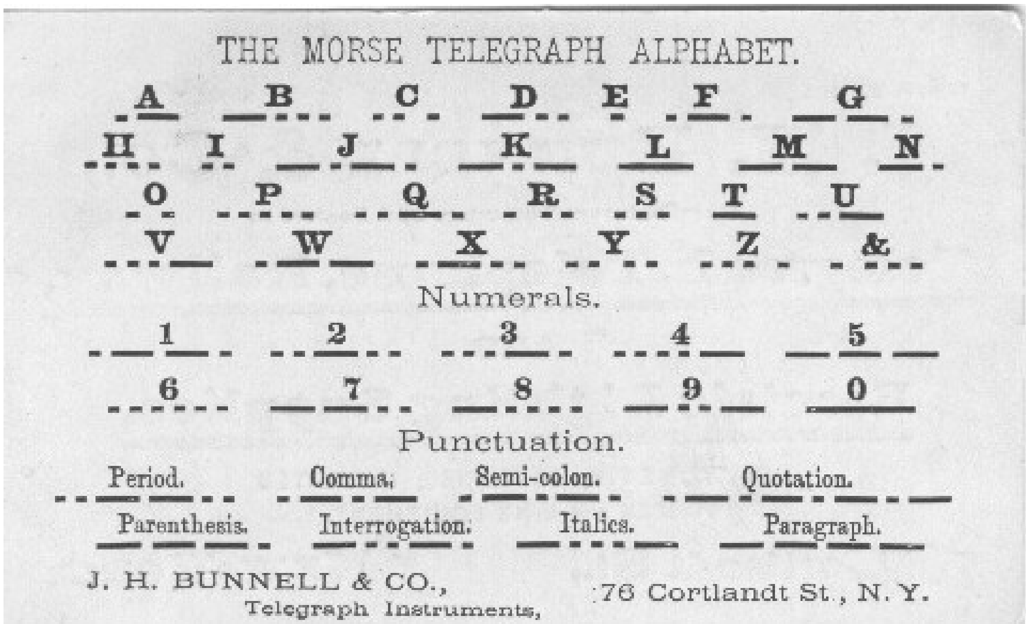
Encoding: Morse Code

This is precisely how **Morse Code** works!

> Approximates **Huffman Coding**, which gives optimal binary codes.

In [19]:
```
Image(filename="images/morse-code.jpg")
```

Out[19]:



Source Coding Theorem

Claude Shannon proved that for discrete noiseless channels:

> It is impossible to encode messages drawn from a distribution p with fewer than $H[p]$ bits, on average.

Here, *bits* refers to *binary digits*, i.e. encoding messages in binary.

> $H[p]$ measures the optimal code length, in bits, for messages drawn from p

Cross Entropy & Relative Entropy

Consider different distributions p and q

- What if we use a code optimal for q to encode messages from p?

For example, suppose our encoding scheme is optimal for German text.

- What if we send English messages instead?
- Certainly, there will be some waste due to different letter frequencies, umlauts, ...

Cross Entropy

The **cross entropy** measures the average number of bits needed to encode messages drawn from p when we use a code optimal for q:

$$H(p, q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x) = -E_p[\log q(x)]$$

Intuitively, $H(p, q) \geq H(p)$. The **relative entropy** is the difference $H(p, q) - H(p)$.

Relative Entropy: Definition

The **relative entropy** or **Kullback-Leibler divergence** of q from p is

$$\begin{aligned} D_{KL}(p||q) &= \sum_{x \in X} p(x) \log \frac{p(x)}{q(x)} \\ &= H(p, q) - H(p) \end{aligned}$$

> Measures the number of *extra* bits needed to encode messages from p if we use a code optimal for q.

Mutual Information: Definition

The **mutual information** between discrete variables X and Y is

$$\begin{aligned} I(X; Y) &= \sum_{y \in Y} \sum_{x \in X} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} \\ &= D_{KL}(p(x, y)||p(x)p(y)) \end{aligned}$$

- If X and Y are independent, $p(x, y) = p(x)p(y)$
- So, $I(X; Y)$ measures how *dependent* X and Y are!
- Related to correlation $\rho(X, Y)$

Example: Collocations & PMI

A **collocation** is a sequence of words that co-occur more often than expected by chance.

- fixed expression familiar to native speakers (hard to translate)
- meaning of the whole is more than the sum of its parts

> See these slides (https://www.eecis.udel.edu/~trnka/CISC889-11S/lectures/philip-pmi.pdf) for more details

Example: Collocation & PMI

Substituting a synonym sounds unnatural:

- "fast food" vs. "quick food"
- "Great Britain" vs. "Good Britain"
- "warm greetings" vs "hot greetings"

> How can we find collocations in a corpus of text?

Example: Collocations & PMI

The **pointwise mutual information** between words x and y is

$$\text{pmi}(x;y) = \log \frac{p(x,y)}{p(x)p(y)}$$

- $p(x)p(y)$ is how frequently we **expect** x and y to co-occur, if they do so independently.
- $p(x,y)$ measures how frequently x and y **actually** occur together

Example: Collocations & PMI

Idea: Rank word pairs by $\mathrm{pmi}(x, y)$ to find collocations!

- $\mathrm{pmi}(x, y)$ is large if x and y co-occur more frequently together than expected

Code: Let's try it on the novel *Crime and Punishment*!

- Pre-computed unigram and bigram counts are found in the `collocations/data` folder

Example: Collocations & PMI

Here we read in the precomputed data. See the notebook in the `collocations` folder for a full implementation.

In [20]:

```
import csv, math;

# file paths
unigram_path = "collocations/data/crime-and-punishment.txt.unigr
ams";
bigram_path = "collocations/data/crime-and-punishment.txt.bigram
s";

# read unigrams into dict
with open(unigram_path) as f:
    reader = csv.reader(f);
    unigrams = { row[0] : int(row[1]) for row in csv.reader(f)};

# read bigrams into dict
with open(bigram_path) as f:
    reader = csv.reader(f);
    bigrams = { (row[0],row[1]) : int(row[2]) for row in csv.rea
der(f)};

# pretty print table
class PrettyTable(object):
        def __init__(self, data, head1, head2, floats=False):
            table = "<table>"
            table += "<thead><th>%s</th><th>%s</th></thead>\n" %
(head1,head2);
            table += "<tbody>\n"
            for bigram,count in data:
                if floats: count = "%0.2f" % count;
                else: count = "%d" % count;

                table += "<tr>"
                table += "<td>%s %s</td>" % bigram;
                table += "<td>%s</td>" % count;
                table += "</tr>\n";

            table += "</tbody></table>"
            self.table = table;

        def _repr_html_(self):
            return self.table;
```

Example: Collocations & PMI

The following code sorts bigrams by pointwise mutual information:

In [30]:
```
# compute pmi
pmi_bigrams = [];

for w1,w2 in bigrams:
    # compute pmi
    actual = bigrams[(w1,w2)];
    expected = unigrams[w1] * unigrams[w2];
    pmi = math.log( actual / expected );
    # filter out infrequent bigrams
    if actual < 15: continue;
    pmi_bigrams.append( ((w1, w2), pmi) );

# sort pmi
pmi_sorted = sorted(pmi_bigrams, key=lambda x: x[1], reverse=True);
```

Example: Collocations & PMI

Here are the most frequent bigrams--these aren't collocations!

In [31]:
```
bigrams_sorted = sorted(bigrams.items(), key=lambda x: x[1], reverse=True);
PrettyTable(bigrams_sorted[:10], "Bigram", "Count")
```

Out[31]:

Bigram	Count
in the	778
of the	598
he was	505
he had	498
to the	488
on the	479
i am	460
at the	459
it was	413
that he	335

Example: Collocations & PMI

Sorting bigrams by PMI, we first get names...

In [33]:
```
PrettyTable(pmi_sorted[1:10], "Collocation", "PMI", floats=True)
```

Out[33]:

Collocation	PMI
andrey semyonovitch	-3.18
nikodim fomitch	-3.18
hay market	-3.48
dmitri prokofitch	-3.87
honoured sir	-4.27
sofya semyonovna	-4.33
marfa petrovna	-4.37
police station	-4.48
rodion romanovitch	-4.57

Example: Collocations & PMI

...then more interesting collocations! This is much more useful than sorting by frequency alone.

In [34]:
```
PrettyTable(pmi_sorted[12:20], "Collocation", "PMI", floats=True)
```

Out[34]:

Collocation	PMI
thank god	-5.20
police office	-5.23
great deal	-5.28
ten minutes	-5.40
good heavens	-5.51
thousand roubles	-5.54
katerina ivanovnas	-5.57
old womans	-5.57

Example: Feature Selection

Mutual information can also be used for **feature selection**.

- In classification, features that *depend* most on the class label C are useful
- So, choose features X_k such that $I(X_k; C)$ is large
- This helps to avoid *overfitting* by ignoring irrelevant features!

> See **[MLAPP]** §3.5.4 for more information

Exponential Families

> Uses material from **[MLAPP]** §9.2 and **[Hero 2008]** §3.5, §4.4.2

Exponential Family: Introduction

We have seen many distributions.

- Bernoulli
- Gaussian
- Exponential
- Gamma

Many of these belong to a more general class called the **exponential family**.

Exponential Family: Introduction

Why do we care?

- only family of distributions with finite-dimensional **sufficient statistics**
- only family of distributions for which **conjugate priors** exist
- makes the least set of assumptions subject to some user-chosen constraints (**Maximum Entropy**)
- core of generalized linear models and **variational inference**

Sufficient Statistics

Recall: A **statistic** $T(\mathcal{D})$ is a function of the observed data $\mathcal{D}$.

- Mean, $T(x_1, \ldots, x_n) = \frac{1}{n}\sum_{k=1}^{n} x_k$
- Variance, maximum, mode, etc.

Sufficient Statistics: Definition

Suppose we have a model P with parameters θ. Then,

> A statistic $T(\mathcal{D})$ is **sufficient** for θ if no other statistic calculated from the same sample provides any additional information about the parameter.

That is, if $T(\mathcal{D}_1) = T(\mathcal{D}_2)$, our estimate of θ given $\mathcal{D}_1$ or $\mathcal{D}_2$ will be the same.

- Mathematically, $P(\theta | T(\mathcal{D}), \mathcal{D}) = P(\theta | T(\mathcal{D}))$ independently of $\mathcal{D}$

Sufficient Statistics: Example

Suppose $X \sim \mathcal{N}(\mu, \sigma^2)$ and we observe $\mathcal{D} = (x_1, \ldots, x_n)$. Let

- $\hat{\mu}$ be the sample mean
- $\hat{\sigma}^2$ be the sample variance

Then $T(\mathcal{D}) = (\hat{\mu}, \hat{\sigma}^2)$ is sufficient for $\theta = (\mu, \sigma^2)$.

- Two samples $\mathcal{D}_1$ and $\mathcal{D}_2$ with the same mean and variance give the same estimate of θ

(we are sweeping some details under the rug)

Exponential Family: Definition

$p(x|\theta)$ has **exponential family form** if:

$$\begin{aligned} p(x|\theta) &= \frac{1}{Z(\theta)} h(x) \exp\left[\eta(\theta)^T \phi(x)\right] \\ &= h(x) \exp\left[\eta(\theta)^T \phi(x) - A(\theta)\right] \end{aligned}$$

- $Z(\theta)$ is the **partition function** for normalization
- $A(\theta) = \log Z(\theta)$ is the **log partition function**
- $\phi(x) \in \mathbb{R}^d$ is a vector of **sufficient statistics**
- $\eta(\theta)$ maps θ to a set of **natural parameters**
- $h(x)$ is a scaling constant, usually $h(x) = 1$

Example: Bernoulli

The Bernoulli distribution can be written as

$$\begin{aligned} \mathrm{Ber}(x|\mu) &= \mu^x (1-\mu)^{1-x} \\ &= \exp[x \log \mu + (1-x) \log(1-\mu)] \\ &= \exp\left[\eta(\mu)^T \phi(x)\right] \end{aligned}$$

where $\eta(\mu) = (\log \mu, \log(1-\mu))$ and $\phi(x) = (x, 1-x)$

- There is a linear dependence between features $\phi(x)$
- This representation is **overcomplete**
- η is not uniquely determined

Example: Bernoulli

Instead, we can find a **minimal** parameterization:

$$\mathrm{Ber}(x|\mu) = (1-\mu)\exp\left[x \log \frac{\mu}{1-\mu}\right]$$

This gives **natural parameters** $\eta = \log \frac{\mu}{1-\mu}$.

- Now, η is unique

Other Examples

Exponential Family Distributions:

- Multivariate normal
- Exponential
- Dirichlet

Non-examples:

- Student t-distribution can't be written in exponential form
- Uniform distribution support depends on the parameters θ

Log-Partition Function

Derivatives of the **log-partition function** $A(\theta)$ yield **cumulants** of the sufficient statistics *(Exercise!)*

- $\nabla_\theta \log p(x|\theta) = E[\phi(x)]$
- $\nabla_\theta^2 \log p(x|\theta) = Cov[\phi(x)]$

This guarantees that $A(\theta)$ is convex!

- Its Hessian is the covariance matrix of X, which is positive-definite.
- Later, this will guarantee a unique global maximum of the likelihood!

Proof of Convexity: First Derivative

$$\begin{aligned}
\frac{dA}{d\theta} &= \frac{d}{d\theta}\left[\log \int exp(\theta\phi(x))h(x)dx\right] \\
&= \frac{\frac{d}{d\theta}\int exp(\theta\phi(x))h(x)dx)}{\int exp(\theta\phi(x))h(x)dx)} \\
&= \frac{\int \phi(x)exp(\theta\phi(x))h(x)dx}{exp(A(\theta)} \\
&= \int \phi(x)\exp[\theta\phi(x) - A(\theta)]h(x)dx \\
&= \int \phi(x)p(x)dx \\
&= E[\phi(x)]
\end{aligned}$$

Proof of Convexity: Second Derivative

$$\begin{aligned}
\frac{d^2A}{d\theta^2} &= \int \phi(x)\exp[\theta\phi(x) - A(\theta)]h(x)(\phi(x) - A'(\theta))dx \\
&= \int \phi(x)p(x)(\phi(x) - A'(\theta))dx \\
&= \int \phi^2(x)p(X)dx - A'(\theta)\int \phi(x)p(x)dx \\
&= E[\phi^2(x)] - E[\phi(x)]^2 \qquad (\because A'(\theta) = E[\phi(x)]) \\
&= Var[\phi(x)]
\end{aligned}$$

Proof of Convexity: Second Derivative

For multi-variate case, we have

$$\frac{\partial^2 A}{\partial\theta_i \partial\theta_j} = E[\phi_i(x)\phi_j(x)] - E[\phi_i(x)]E[\phi_j(x)]$$

and hence,

$$\nabla^2 A(\theta) = Cov[\phi(x)]$$

Since covariance is positive definite, we have $A(\theta)$ convex as required.

Exponential Family: Likelihood

For data $\mathcal{D} = (x_1, \ldots, x_N)$, the likelihood is

$$p(\mathcal{D}|\theta) = \left[\prod_{k=1}^{N} h(x_k)\right] Z(\theta)^{-N} \exp\left[\eta(\theta)^T \sum_{k=1}^{N} \phi(x_k)\right]$$

The sufficient statistics are now N and $\phi(\mathcal{D}) = \sum_{k=1}^{N} \phi(x)$.

- **Bernoulli:** N and $\phi = \#Heads$
- **Normal:** N and $\phi = [\sum_k x_k, \sum_k x_k^2]$

Pitman-Koopman-Darmois Theorem

> Among families of distributions $P(x|\theta)$ whose support does not vary with the parameter θ, only in exponential families is there a sufficient statistic $T(x_1, \ldots, x_N)$ whose dimension remains bounded as the sample size N increases.

Exponential Family: MLE

For natural parameters θ and data $\mathcal{D} = (x_1, \ldots, x_N)$,

$$\log p(\mathcal{D}|\theta) = \eta^T \phi(\mathcal{D}) - NA(\theta)$$

Since $-A(\theta)$ is concave and $\theta^T \phi(\mathcal{D})$ linear,

- the log-likelihood is concave
- there is a unique global maximum!

Exponential Family: MLE

To find the maximum, recall $\nabla_\theta \log p(x|\theta) = E[\phi(x)]$, so

$$\nabla_\theta \log p(\mathcal{D}|\theta) = \phi(\mathcal{D}) - NE[\phi(X)] = 0$$
$$\implies E[\phi(X)] = \frac{\phi(\mathcal{D})}{N} = \frac{1}{N} \sum_{k=1}^{N} \phi(x_k)$$

At the MLE $\hat{\theta}_{MLE}$, the empirical average of sufficient statistics equals their expected value.

- this is called **moment matching**

Exponential Family: MLE

As an example, consider the Bernoulli distribution

- Sufficient statistic N, $\phi(\mathcal{D}) = \#Heads$

$$\hat{\mu}_{MLE} = \frac{\#Heads}{N}$$

Bayes for Exponential Family

Exact Bayesian analysis is considerably simplified if the prior is **conjugate** to the likelihood.

- Simply, this means that prior $p(\mathcal{D}|\tau)$ has the same form as likelihood $p(\mathcal{D}|\theta)$.

This requires likelihood to have finite sufficient statistics

- Exponential family to the rescue!

Likelihood

Likelihood:

$$p(\mathcal{D}|\theta) \propto g(\theta)^N \exp[\eta(\theta)^T s_N]$$
$$s_N = \sum_{i=1}^{N} s(x_i)$$

In terms of canonical parameters:

$$p(\mathcal{D}|\eta) \propto \exp[N\eta^T \bar{s} - NA(\eta)]$$
$$\bar{s} = \frac{1}{N} s_N$$

Prior

$$p(\theta|\nu_0, \tau_0) \propto g(\theta)^{\nu_0} \exp[\eta(\theta)^T \tau_0]$$

- Denote $\tau_0 = \nu_0 \bar{\tau}_0$ to separate out the size of the **prior pseudo-data**, ν_0 , from the mean of the sufficient statistics on this pseudo-data, τ_0 . Hence,

$$p(\theta|\nu_0, \bar{\tau}_0) \propto \exp[\nu_0 \eta^T \bar{\tau}_0 - \nu_0 A(\eta)]$$

Prior: Example

$$
\begin{aligned}
p(\theta|\nu_0, \tau_0) &\propto (1-\theta)^{\nu_0} \exp[\tau_0 \log(\frac{\theta}{1-\theta})] \\
&= \theta^{\tau_0} (1-\theta)^{\nu_0 - \tau_0}
\end{aligned}
$$

Define $\alpha = \tau_0 + 1$ and $\beta = \nu_0 - \tau_0 + 1$ to see that this is a **beta distribution**.

Posterior

Posterior:

$$
p(\theta|\mathcal{D}) = p(\theta|\nu_N, \tau_N) = p(\theta|\nu_0 + N, \tau_0 + s_N)
$$

Note that we obtain **hyper-parameters** by adding. Hence,

$$
\begin{aligned}
p(\eta|\mathcal{D}) &\propto \exp[\eta^T(\nu_0 \bar{\tau}_0 + N\bar{s}) - (\nu_0 + N)A(\eta)] \\
&= p(\eta|\nu_0 + N, \frac{\nu_0 \bar{\tau}_0 + N\bar{s}}{\nu_0 + N})
\end{aligned}
$$

- *posterior hyper-parameters are a convex combination of the prior mean hyper-parameters and the average of the sufficient statistics.*