Scalable Machine Learning

2. Statistics

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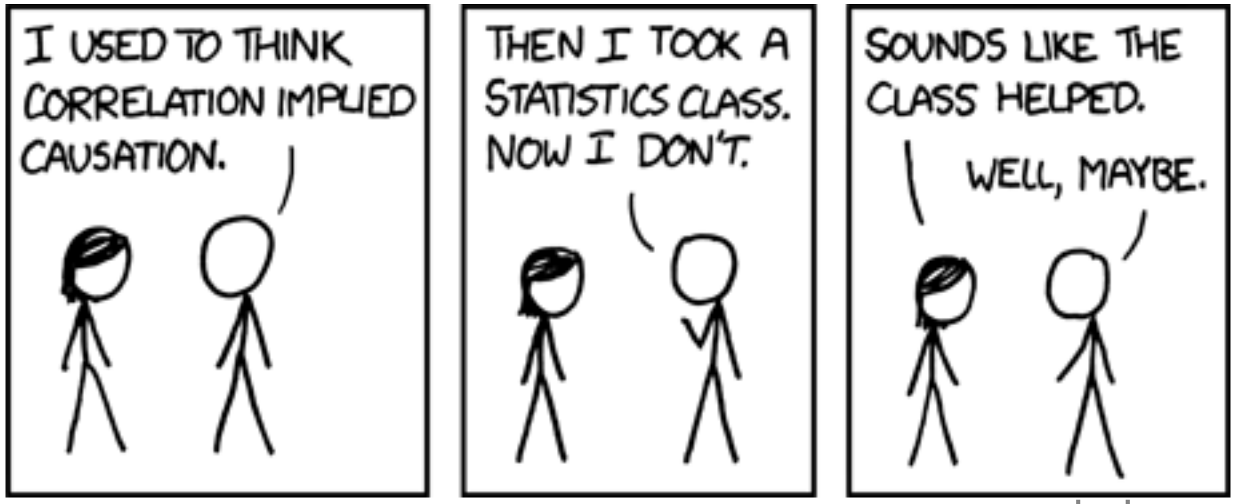
Stat 260 SP 12



xkcd.com

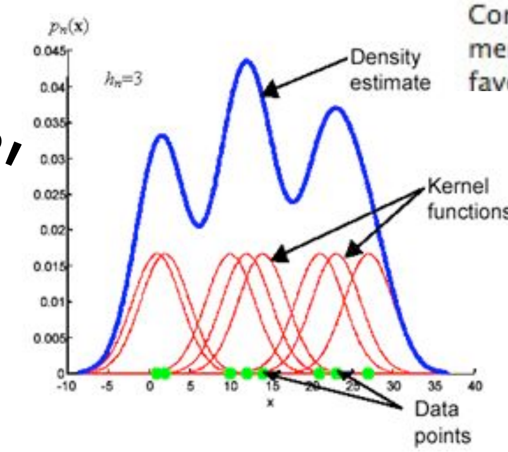
2. Statistics

Essential tools for data analysis

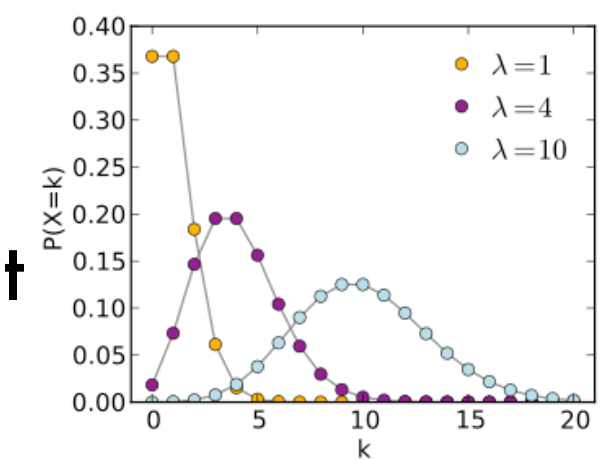
Statistics

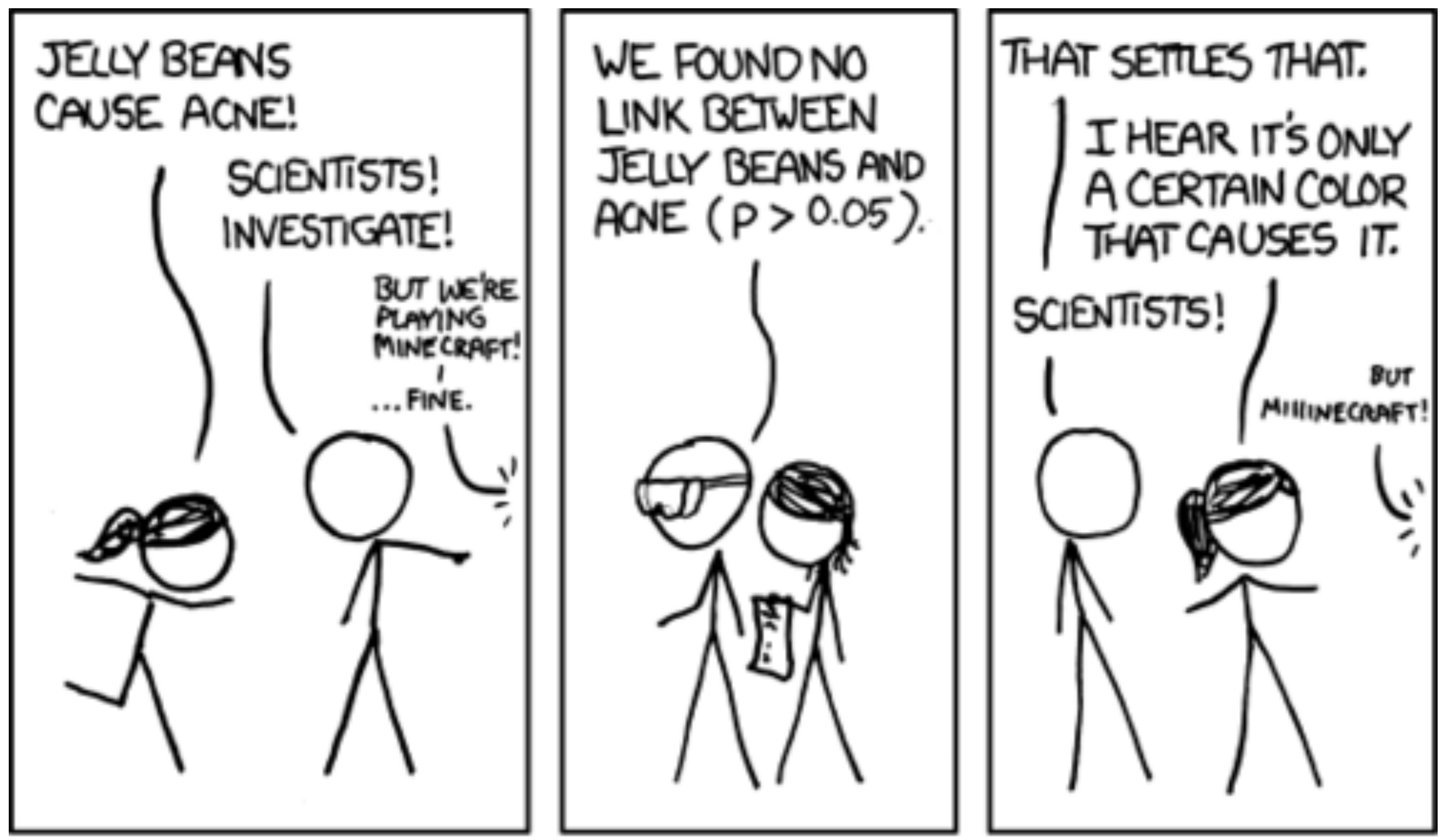
- Probabilities
  - Bayes rule, Dependence, independence, conditional probabilities
  - Priors, Naive Bayes classifier
- Tail bounds
  - Chernoff, Hoeffding, Chebyshev, Gaussian
  - A/B testing

- Kernel density estimation
  - Parzen windows, Nearest neighbors, Watson-Nadaraya estimator

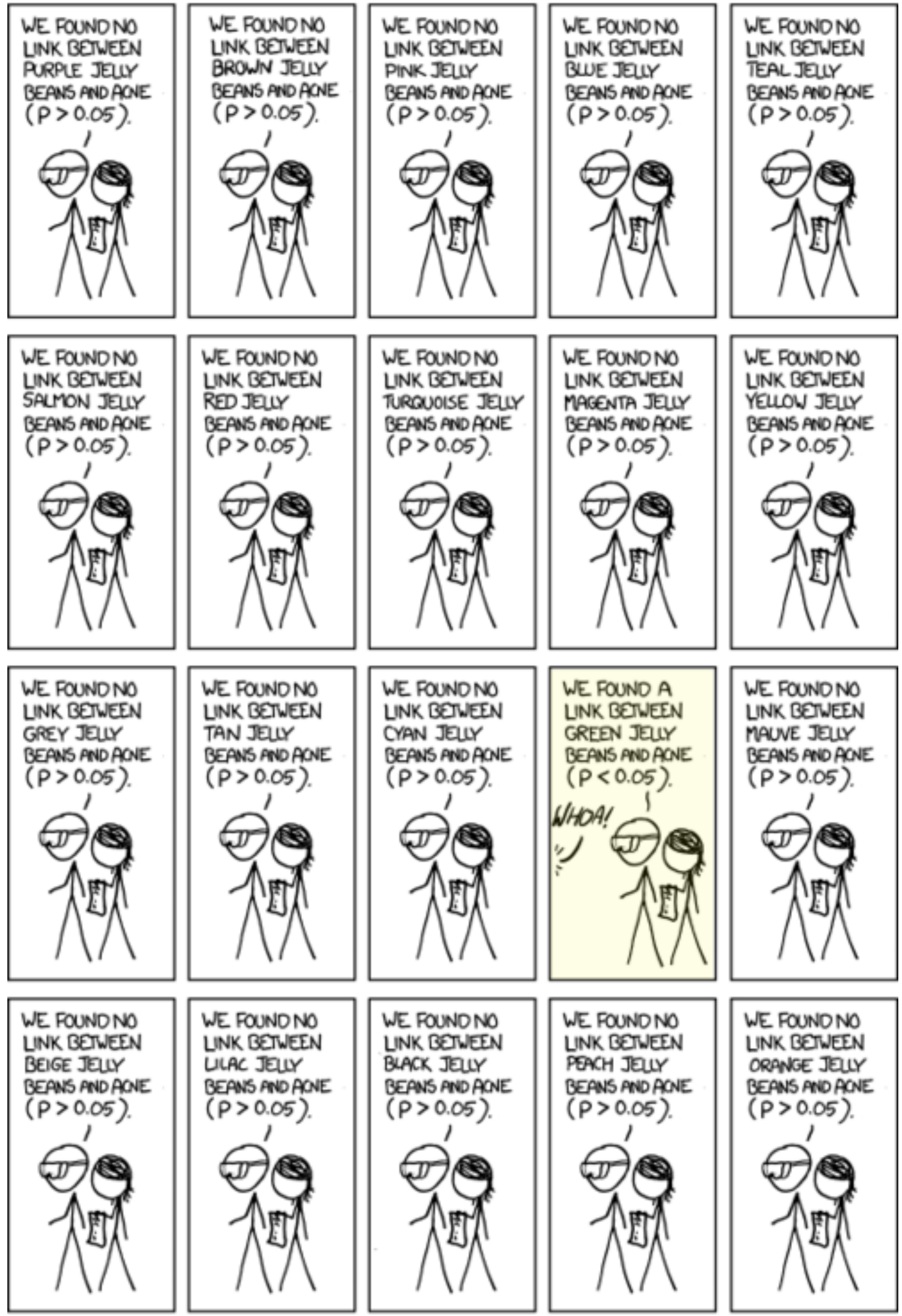


- Exponential families
  - Gaussian, multinomial, Poisson
  - Conjugate distributions and smoothing, integrating out

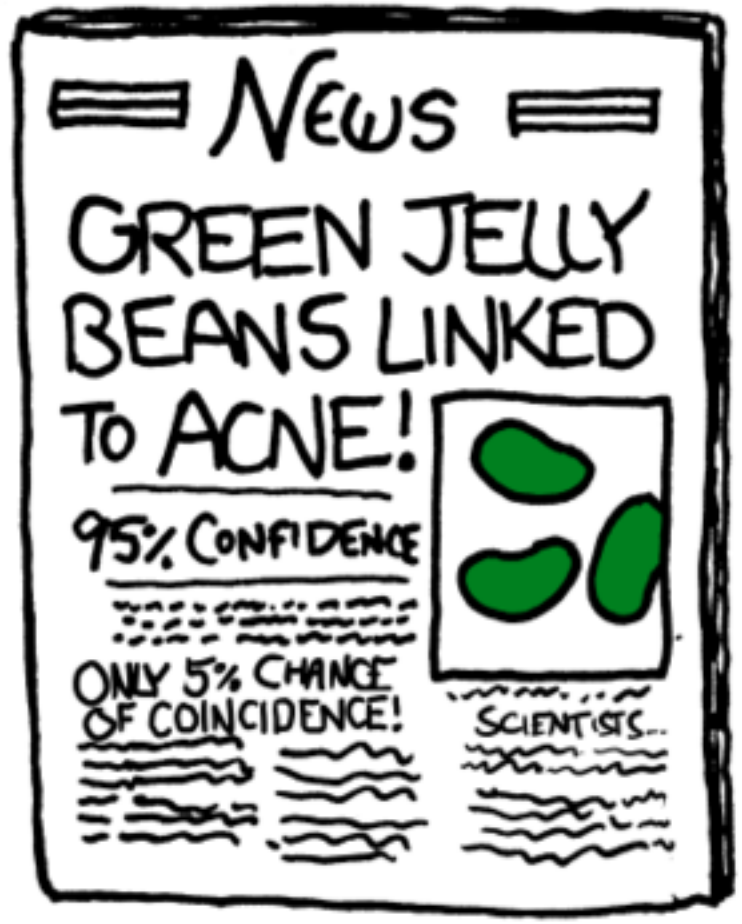



JELLY BEANS CAUSE ACNE!
SCIENTISTS! INVESTIGATE!
BUT WE'RE PLAYING MINECRAFT!
...FINE.
WE FOUND NO LINK BETWEEN JELLY BEANS AND ACNE (P > 0.05).
THAT SETTLES THAT.
I HEAR IT'S ONLY A CERTAIN COLOR THAT CAUSES IT.
SCIENTISTS!
BUT MIIINECRAFT!

xkcd.com


WE FOUND NO LINK BETWEEN PURPLE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN BROWN JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN PINK JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN BLUE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN TEAL JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN SALMON JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN RED JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN TURQUOISE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN MAGENTA JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN YELLOW JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN GREY JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN TAN JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN CYAN JELLY BEANS AND ACNE (P > 0.05).
WE FOUND A LINK BETWEEN GREEN JELLY BEANS AND ACNE (P < 0.05).
WHOA!
WE FOUND NO LINK BETWEEN MAUVE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN BEIGE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN LILAC JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN BLACK JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN PEACH JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN ORANGE JELLY BEANS AND ACNE (P > 0.05).

xkcd.com


NEWS
GREEN JELLY BEANS LINKED TO ACNE!
95% CONFIDENCE
ONLY 5% CHANCE OF COINCIDENCE!
SCIENTISTS...

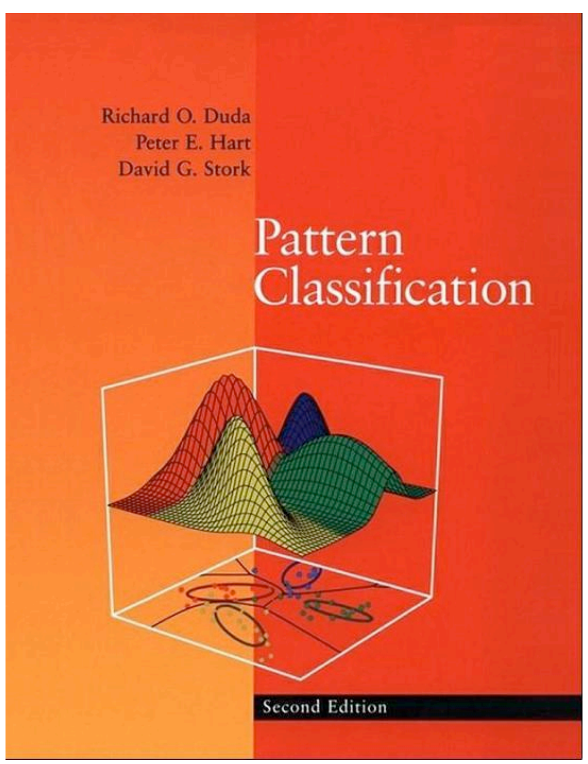
xkcd.com

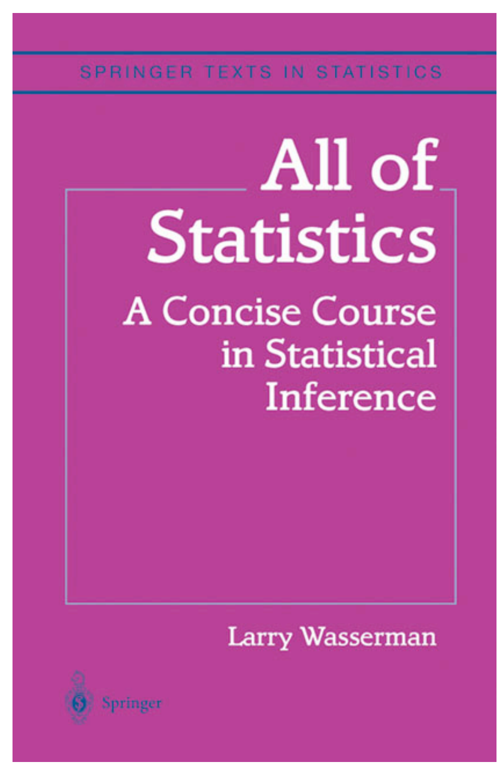
2.1 Probabilities

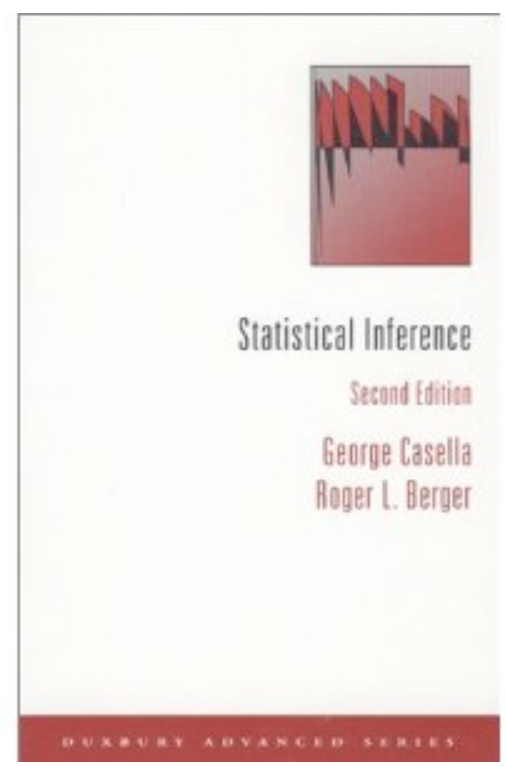
Bayes

Kolmogorov

Statistics 101







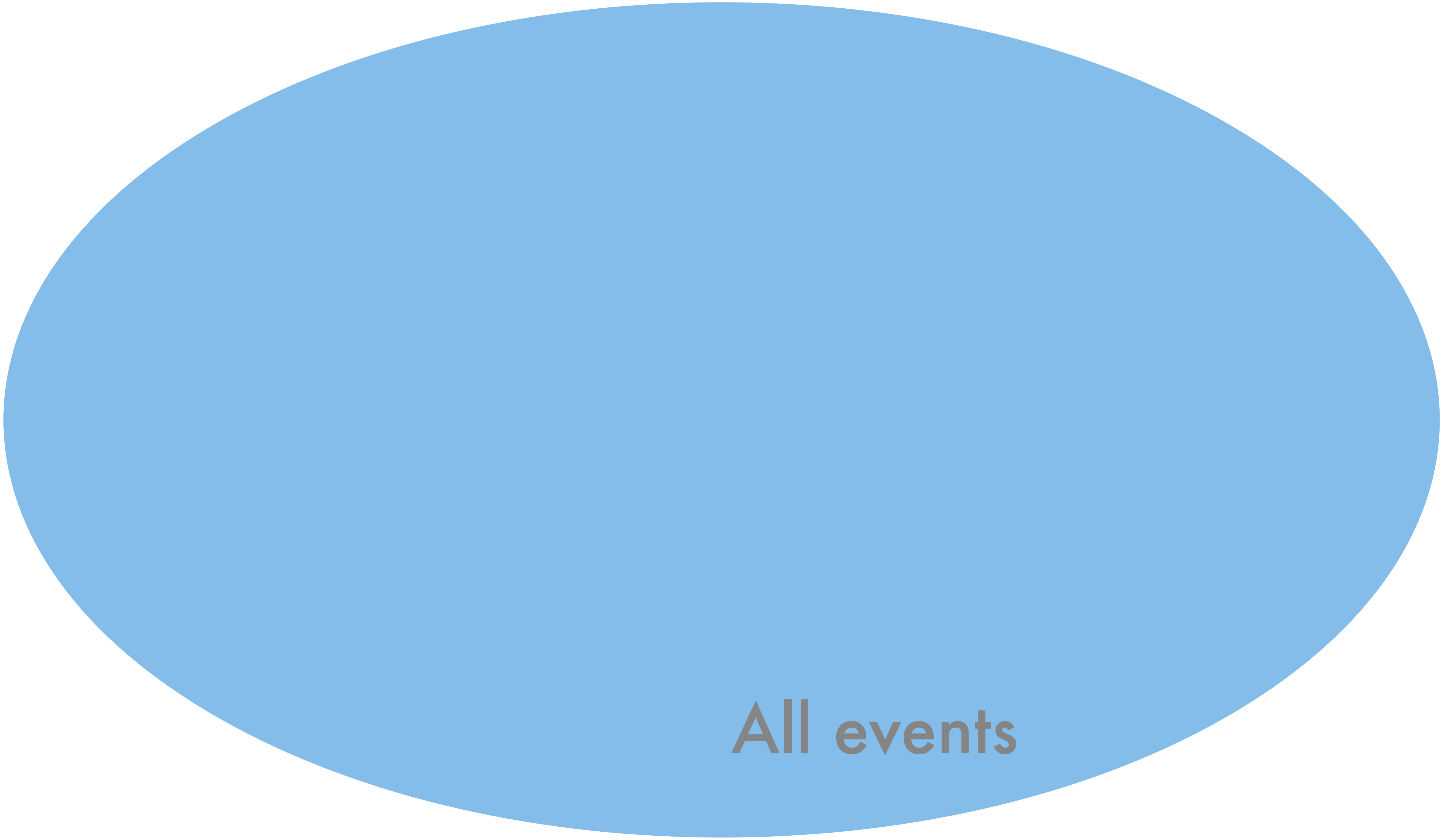
Probability

- Space of events X
  - server working; slow response; server broken
  - income of the user (e.g. $95,000)
  - query text for search (e.g. “statistics tutorial”)
- Probability axioms (Kolmogorov)

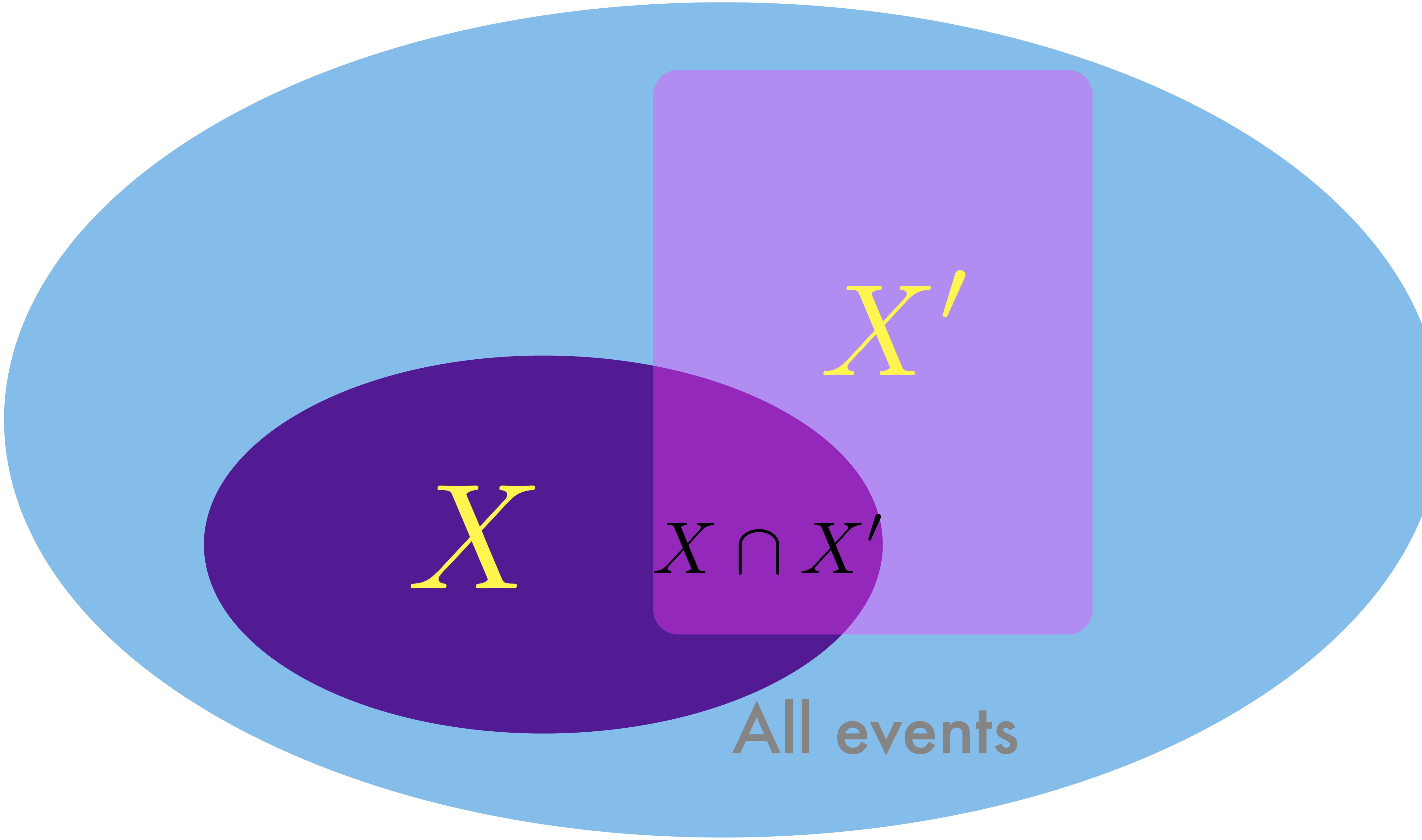
$$\Pr(X) \in [0, 1], \Pr(\mathcal{X}) = 1$$
$$\Pr(\cup_i X_i) = \sum_i \Pr(X_i) \text{ if } X_i \cap X_j = \emptyset$$

- Example queries
  - P(server working) = 0.999
  - P(90,000 < income < 100,000) = 0.1

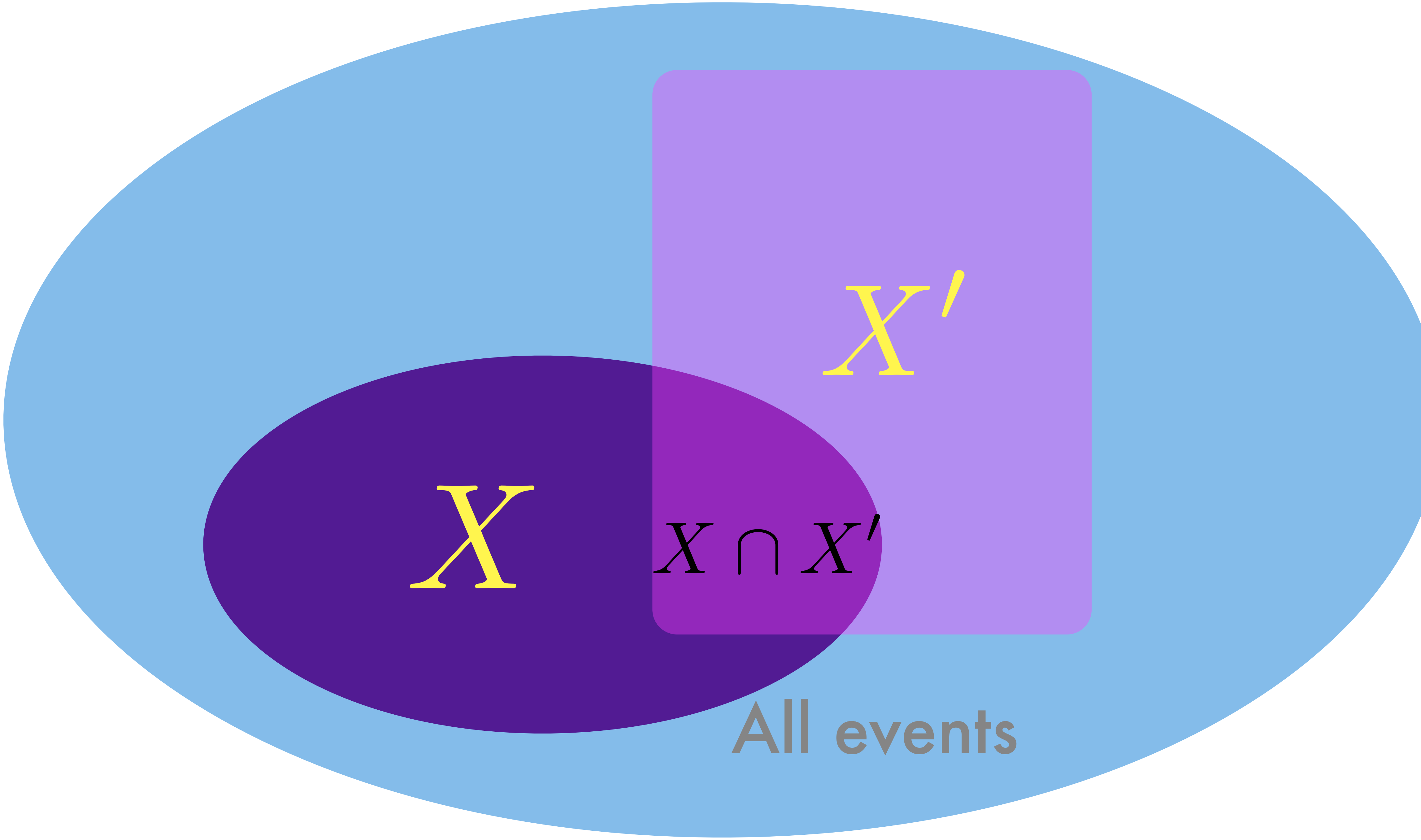
Venn Diagram



Venn Diagram



Venn Diagram



$$\Pr(X \cup X') = \Pr(X) + \Pr(X') - \Pr(X \cap X')$$

(In)dependence

- Independence $\Pr(x, y) = \Pr(x) \cdot \Pr(y)$
  - Login behavior of two users (approximately)
  - Disk crash in different colos (approximately)

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  - Queries
  - News stream / Buzz / Tweets
  - IM communication
  - Russian Roulette

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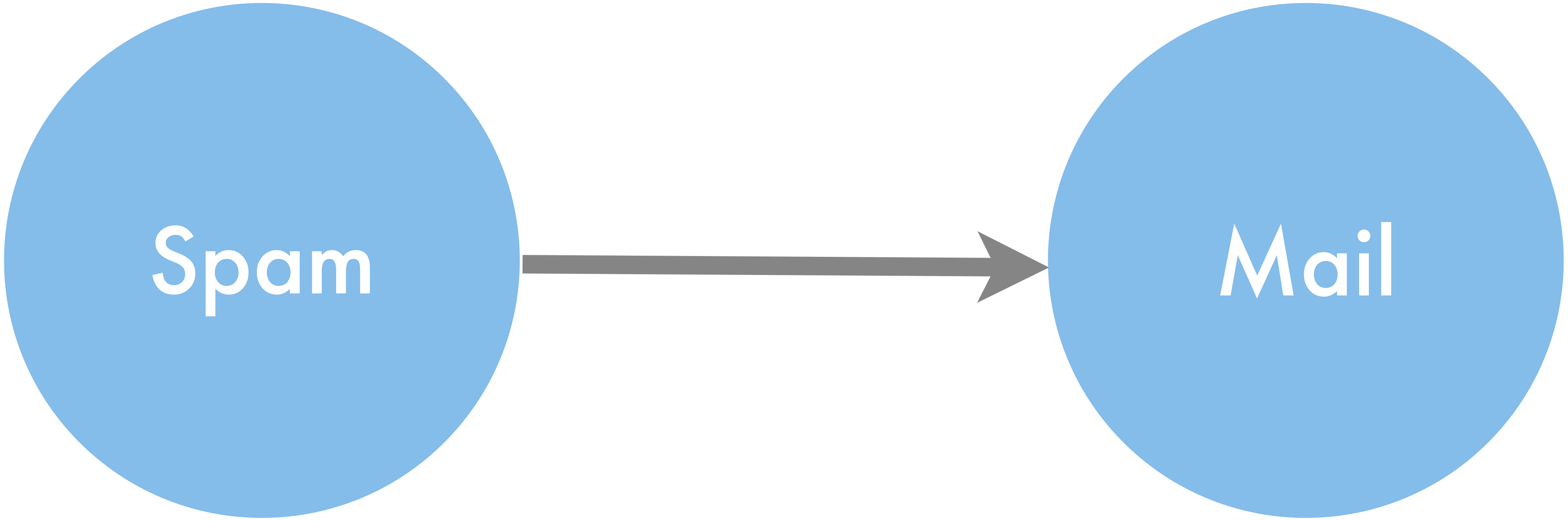
Everywhere!

A Graphical Model



p(spam, mail) = p(spam) p(mail|spam)

Bayes Rule

- Joint Probability

$$\Pr(X, Y) = \Pr(X|Y)\Pr(Y) = \Pr(Y|X)\Pr(X)$$

- Bayes Rule

$$\Pr(X|Y) = \frac{\Pr(Y|X) \cdot \Pr(X)}{\Pr(Y)}$$

- Hypothesis testing
- Reverse conditioning

AIDS test (Bayes rule)

- Data
  - Approximately 0.1% are infected
  - Test detects all infections
  - Test reports positive for 1% healthy people
- Probability of having AIDS if test is positive

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$$
\begin{aligned}
\Pr(a=1|t) &= \frac{\Pr(t|a=1)\cdot\Pr(a=1)}{\Pr(t)} \\
&= \frac{\Pr(t|a=1)\cdot\Pr(a=1)}{\Pr(t|a=1)\cdot\Pr(a=1)+\Pr(t|a=0)\cdot\Pr(a=0)} \\
&= \frac{1\cdot 0.001}{1\cdot 0.001+0.01\cdot 0.999} = 0.091
\end{aligned}
$$

Improving the diagnosis

Improving the diagnosis

- Use a follow-up test
  - Test 2 reports positive for 90% infections
  - Test 2 reports positive for 5% healthy people

$$\frac{0.01 \cdot 0.05 \cdot 0.999}{1 \cdot 0.9 \cdot 0.001 + 0.01 \cdot 0.05 \cdot 0.999} = 0.357$$

Improving the diagnosis

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- Why can't we use Test 1 twice?
  Outcomes are **not** independent but tests 1 and 2 are **conditionally independent**

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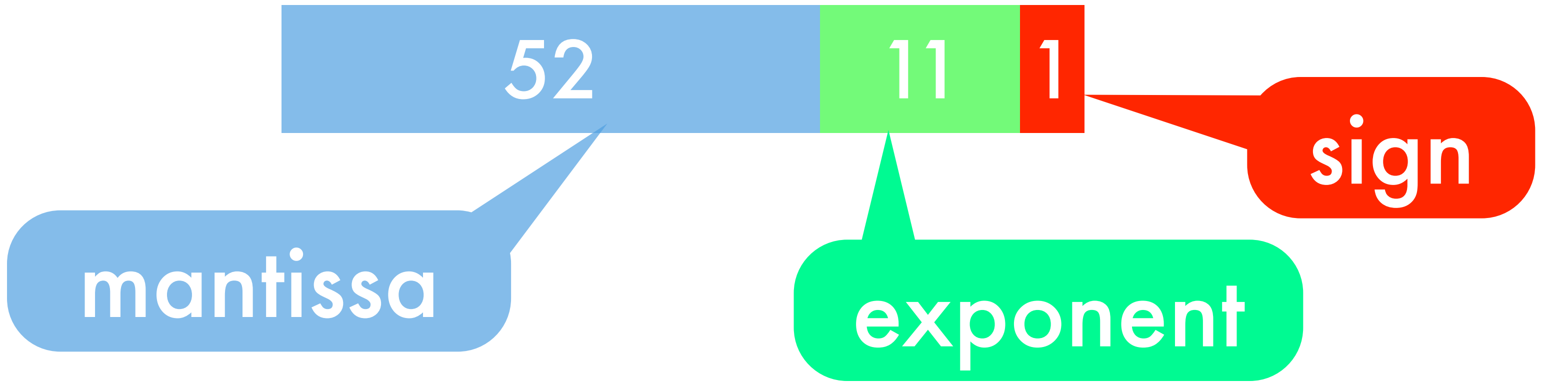
- Why can't we use Test 1 twice?
  Outcomes are **not** independent but tests 1 and 2 are **conditionally independent**

$$p(t_1, t_2|a) = p(t_1|a) \cdot p(t_2|a)$$

Logarithms are good

- Floating point numbers



$$\pi = \log p$$

- Probabilities can be very small. In particular products of many probabilities. Underflow!
- Store data in mantissa, not exponent

$$\prod_i p_i \to \sum_i \pi_i \qquad \sum_i p_i \to \max \pi + \log \sum_i \exp \left[\pi_i - \max \pi\right]$$

- Known bug e.g. in Mahout Dirichlet clustering

Application: Naive Bayes

Naive Bayes Spam Filter

Naive Bayes Spam Filter

- Key assumption
  Words occur independently of each other given the label of the document

$$p(w_1, \ldots, w_n|\text{spam}) = \prod_{i=1}^{n} p(w_i|\text{spam})$$

Naive Bayes Spam Filter

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$$p(w_1, \ldots, w_n | \text{spam}) = \prod_{i=1}^{n} p(w_i | \text{spam})$$

- Spam classification via Bayes Rule

$$p(\text{spam} | w_1, \ldots, w_n) \propto p(\text{spam}) \prod_{i=1}^{n} p(w_i | \text{spam})$$

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$$p(\text{spam}|w_1, \ldots, w_n) \propto p(\text{spam}) \prod_{i=1}^{n} p(w_i|\text{spam})$$

- Parameter estimation
  Compute spam probability and word distributions for spam and ham

Naive Bayes Spam Filter

Equally likely phrases

- Get rich quick. Buy UCB stock.
- Buy Viagra. Make your UCB experience last longer.
- You deserve a PhD from UCB.
  We recognize your expertise.

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- You deserve a PhD from UCB.
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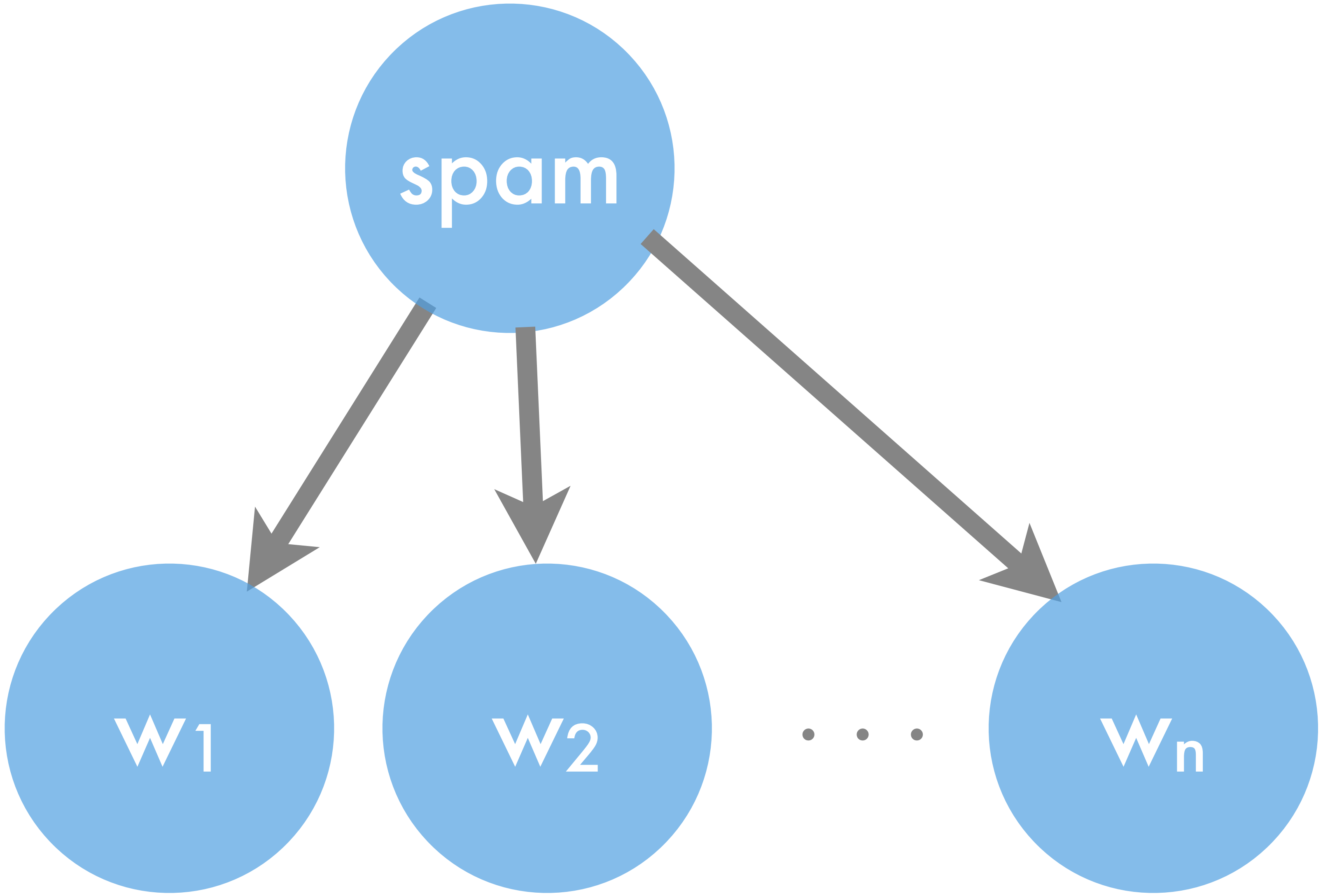
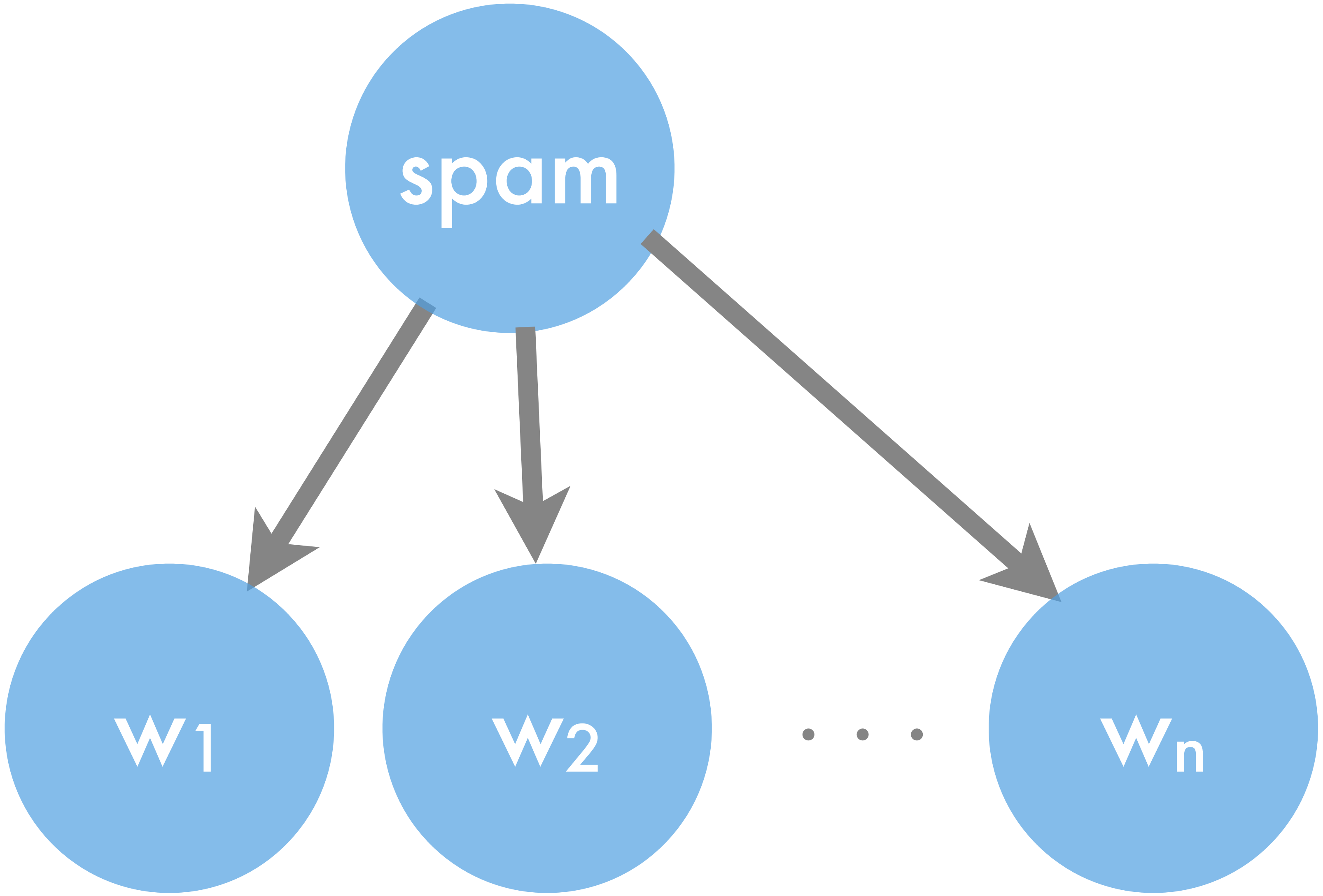
- Make your rich UCB PhD experience last longer.

A Graphical Model



A Graphical Model



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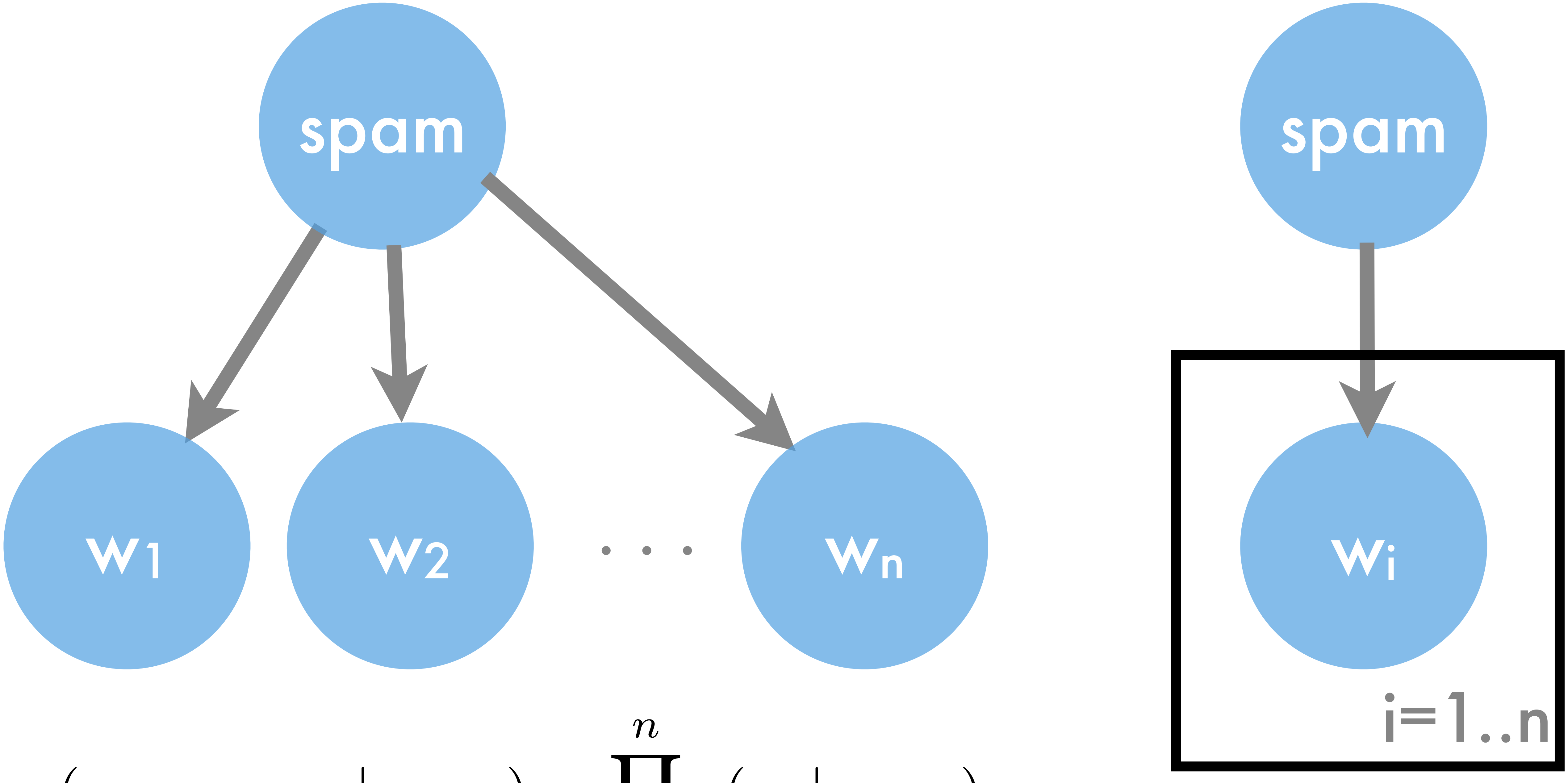

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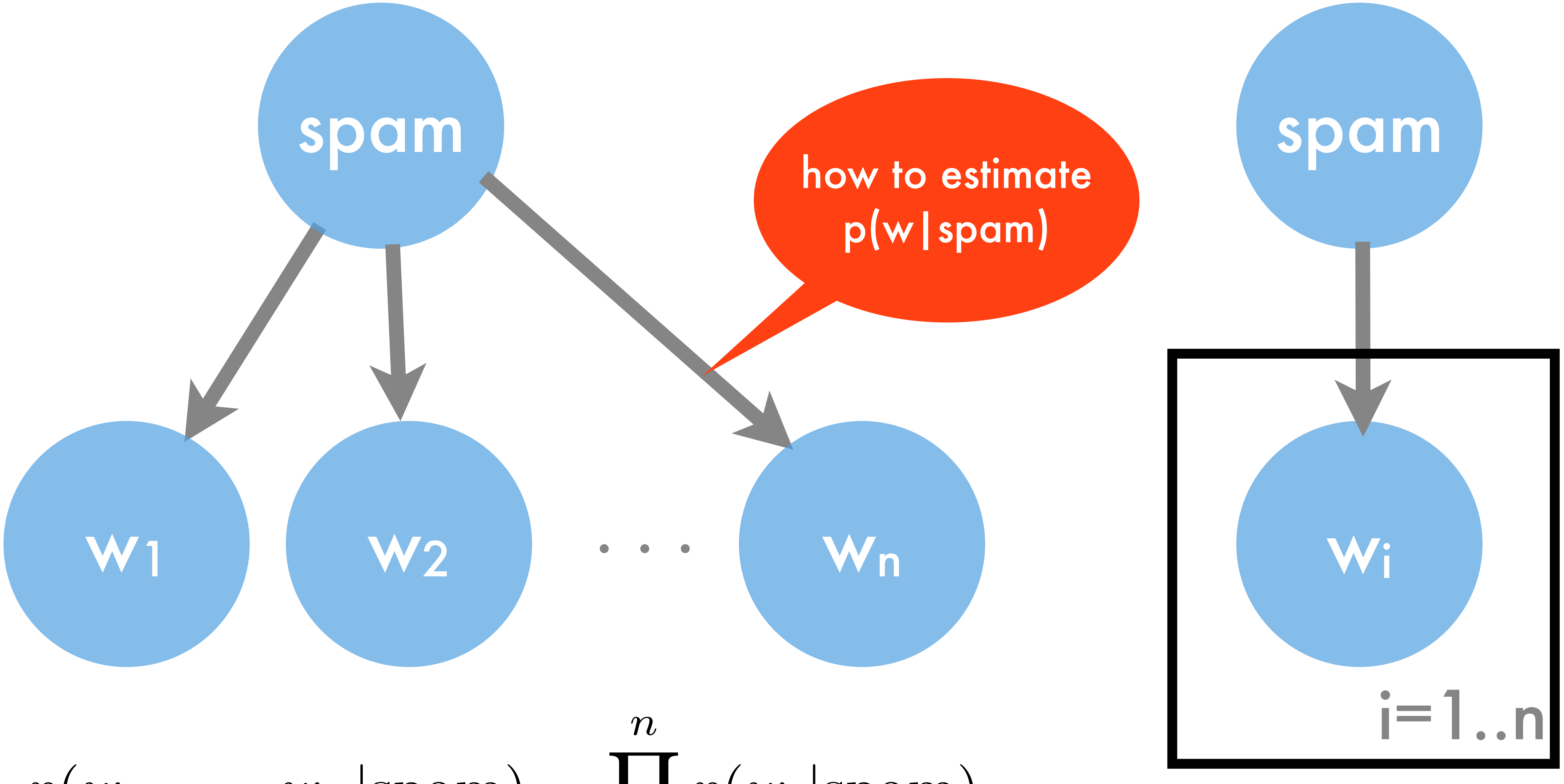

$$p(w_1, \ldots, w_n|\text{spam}) = \prod_{i=1}^{n} p(w_i|\text{spam})$$

Naive Bayes Spam Filter

- Data
  - Emails (headers, body, metadata)
  - Labels (spam/ham)
    assume that users actually label all mails
- Processing capability
  - Billions of e-mails
  - 1000s of servers
- Need to estimate $p(y)$, $p(x_i|y)$
  - Compute distribution of x_i for every y
  - Compute distribution of y

this is a gross simplification

- date
- time
- recipient path
- IP number
- sender
- encoding
- many more features

```
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Received: by 10.216.47.73 with SMTP id s51cs361171web;
        Tue, 3 Jan 2012 14:17:53 -0800 (PST)
Received: by 10.213.17.145 with SMTP id s17mr2519891eba.147.1325629071725;
        Tue, 03 Jan 2012 14:17:51 -0800 (PST)
Return-Path: <alex+caf_=alex.smola=gmail.com@smola.org>
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        (version=TLSv1/SSLv3 cipher=OTHER);
        Tue, 03 Jan 2012 14:17:51 -0800 (PST)
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Subject: CS 281B. Advanced Topics in Learning and Decision Making
From: Tim Althoff <althoff@eecs.berkeley.edu>
```
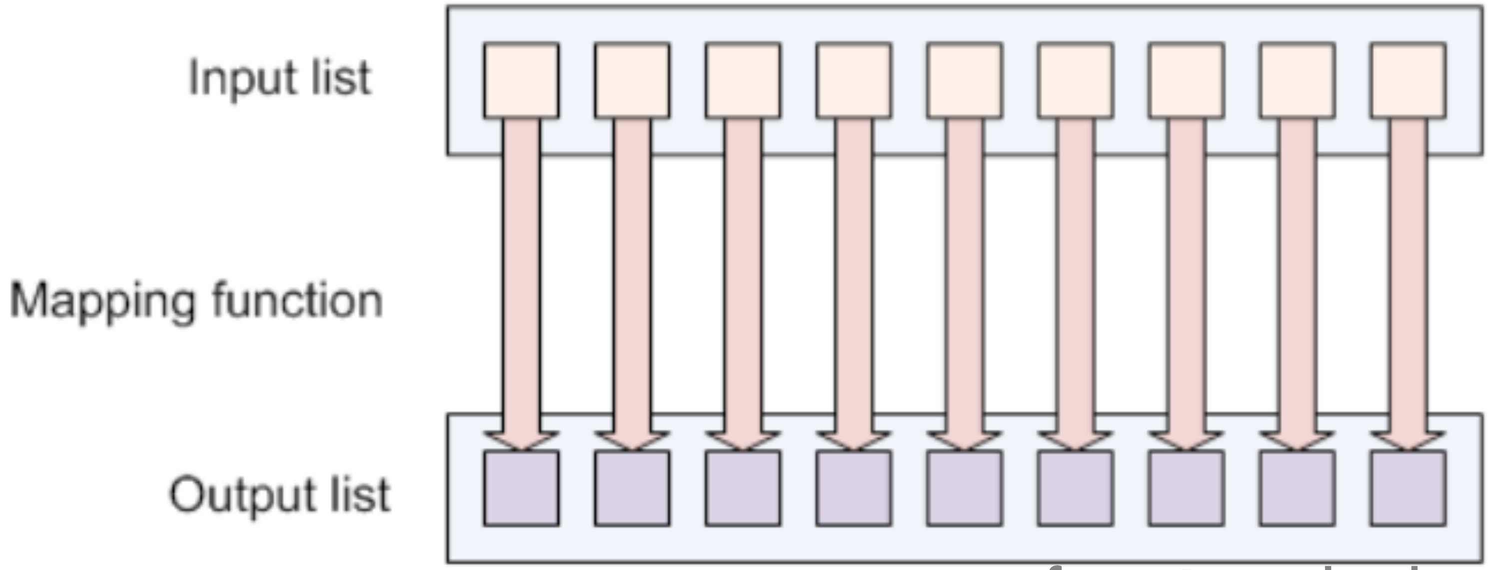
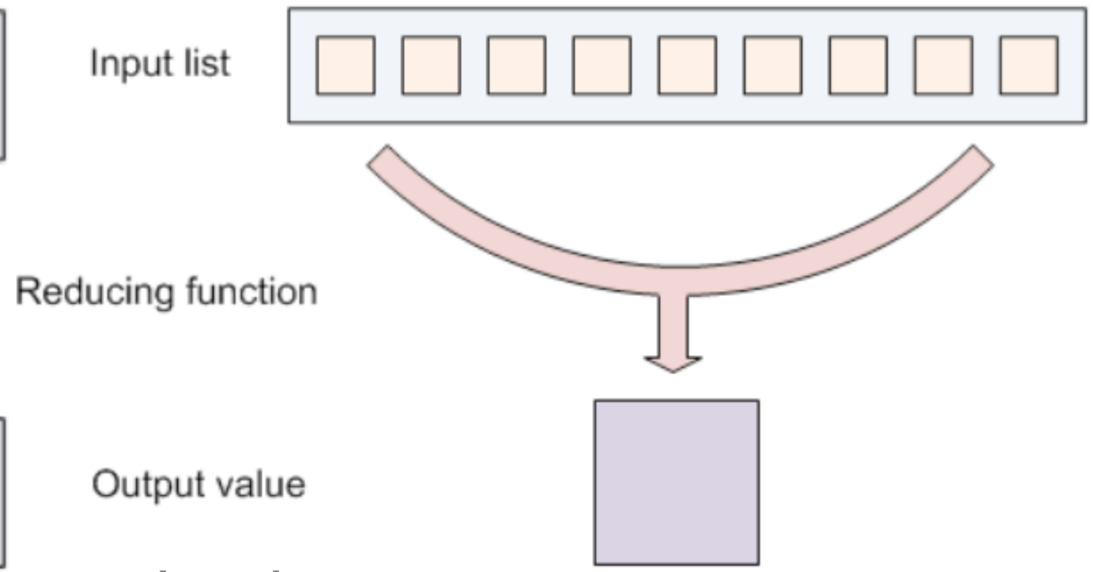

Recall - Map Reduce

- 1000s of (faulty) machines
- Lots of jobs are mostly embarrassingly parallel (except for a sorting/transpose phase)
- Functional programming origins
  - Map(key,value)
    processes each (key,value) pair and outputs a new (key,value) pair
  - Reduce(key,value)
    reduces all instances with same key to aggregate





from Ramakrishnan, Sakrejda, Canon, DoE 2011

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- Example - extremely naive wordcount
  - Map(docID, document)
    for each document emit many (wordID, count) pairs
  - Reduce(wordID, count)
    sum over all counts for given wordID and emit (wordID, aggregate)

Naive NaiveBayes Classifier

- Two classes (spam/ham)
- Binary features (e.g. presence of $$$, viagra)
- Simplistic Algorithm
  - Count occurrences of feature for spam/ham
  - Count number of spam/ham mails

feature probability

spam probability

$$p(x_i = \mathrm{TRUE}|y) = \frac{n(i,y)}{n(y)} \text{ and } p(y) = \frac{n(y)}{n}$$

$$p(y|x) \propto \frac{n(y)}{n} \prod_{i:x_i=\mathrm{TRUE}} \frac{n(i,y)}{n(y)} \prod_{i:x_i=\mathrm{FALSE}} \frac{n(y)-n(i,y)}{n(y)}$$

Naive NaiveBayes Classifier

what if n(i,y)=n(y)?

what if n(i,y)=0?

$$p(y|x) \propto \frac{n(y)}{n} \prod_{i:x_i=\mathrm{TRUE}} \frac{n(i,y)}{n(y)} \prod_{i:x_i=\mathrm{FALSE}} \frac{n(y)-n(i,y)}{n(y)}$$

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Simple Algorithm

- For each document (x,y) do
  - Aggregate label counts given y
  - For each feature x_i in x do
    - Aggregate statistic for (x_i, y) for each y
- For y estimate distribution p(y)
- For each (x_i,y) pair do
  Estimate distribution $p(x_i|y)$, e.g. Parzen Windows, Exponential family (Gauss, Laplace, Poisson, ...), Mixture
- Given new instance compute

$$p(y|x) \propto p(y) \prod_j p(x_j|y)$$

Simple Algorithm

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pass over all data

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trivially parallel

- Given new instance compute

$$p(y|x) \propto p(y) \prod_j p(x_j|y)$$

MapReduce Algorithm

- Map(document (x,y))
  - For each mapper for each feature x_i in x do
    - Aggregate statistic for (x_i, y) for each y
  - Send statistics (key = (x_i,y), value = counts) to reducer
- Reduce(x_i, y)
  - Aggregate over all messages from mappers
  - Estimate distribution $p(x_i|y)$, e.g. Parzen Windows, Exponential family (Gauss, Laplace, Poisson, ...), Mixture
  - Send coordinate-wise model to global storage
- Given new instance compute

$$p(y|x) \propto p(y) \prod_j p(x_j|y)$$

MapReduce Algorithm

- Map(document (x,y))
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local per chunkserver

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  - Send coordinate-wise model to global storage

only aggregates needed

- Given new instance compute

$$p(y|x) \propto p(y) \prod_j p(x_j|y)$$

Estimating Probabilities

Binomial Distribution

- Two outcomes (head, tail); (0,1)
- Data likelihood

$$p(X;\pi) = \pi^{n_1}(1-\pi)^{n_0}$$

- Maximum Likelihood Estimation
  - Constrained optimization problem $\pi \in [0,1]$
  - Incorporate constraint via $p(x;\theta) = \frac{e^{x\theta}}{1+e^{\theta}}$
  - Taking derivatives yields

$$\theta = \log \frac{n_1}{n_0 + n_1} \iff p(x=1) = \frac{n_1}{n_0+n_1}$$

... in detail ...

$$p(X;\theta) = \prod_{i=1}^{n} p(x_i;\theta) = \prod_{i=1}^{n} \frac{e^{\theta x_i}}{1+e^{\theta}}$$

$$\Longrightarrow \log p(X;\theta) = \theta \sum_{i=1}^{n} x_i - n \log\left[1+e^{\theta}\right]$$

$$\Longrightarrow \partial_\theta \log p(X;\theta) = \sum_{i=1}^{n} x_i - n \frac{e^{\theta}}{1+e^{\theta}}$$

$$\Longleftrightarrow \frac{1}{n} \sum_{i=1}^{n} x_i = \frac{e^{\theta}}{1+e^{\theta}} = p(x=1)$$

... in detail ...

$$p(X;\theta) = \prod_{i=1}^{n} p(x_i;\theta) = \prod_{i=1}^{n} \frac{e^{\theta x_i}}{1+e^{\theta}}$$

$$\implies \log p(X;\theta) = \theta \sum_{i=1}^{n} x_i - n \log\left[1+e^{\theta}\right]$$

$$\implies \partial_\theta \log p(X;\theta) = \sum_{i=1}^{n} x_i - n \frac{e^{\theta}}{1+e^{\theta}}$$

$$\iff \frac{1}{n}\sum_{i=1}^{n} x_i = \frac{e^{\theta}}{1+e^{\theta}} = p(x=1)$$

empirical probability of x=1

Discrete Distribution

- n outcomes (e.g. USA, Canada, India, UK, NZ)
- Data likelihood

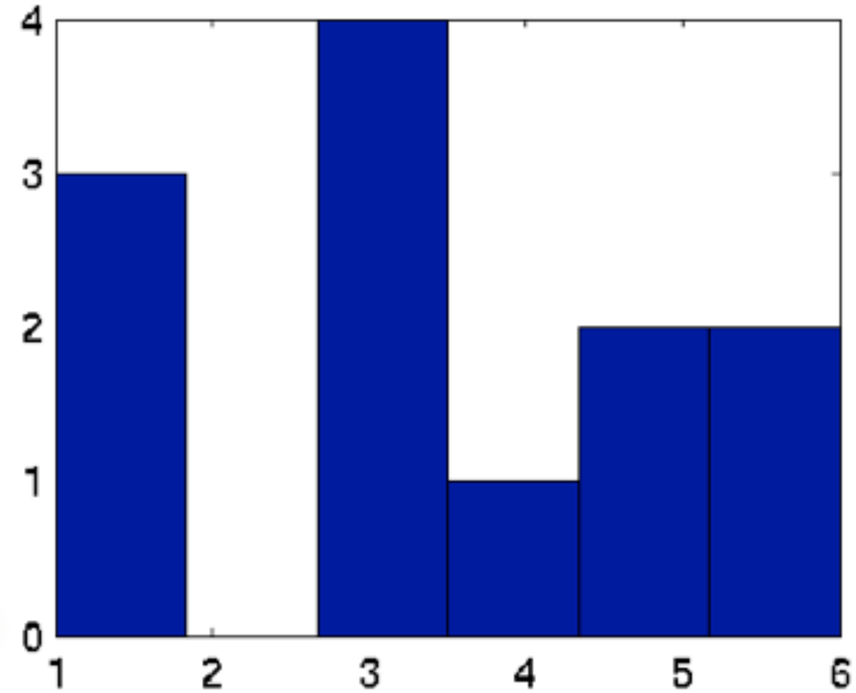
$$p(X; \pi) = \prod_i \pi_i^{n_i}$$

- Maximum Likelihood Estimation
  - Constrained optimization problem ... or ...
  - Incorporate constraint via $p(x; \theta) = \frac{\exp \theta_x}{\sum_{x'} \exp \theta_{x'}}$
  - Taking derivatives yields

$$\theta_i = \log \frac{n_i}{\sum_j n_j} \iff p(x = i) = \frac{n_i}{\sum_j n_j}$$

Tossing a Dice

12



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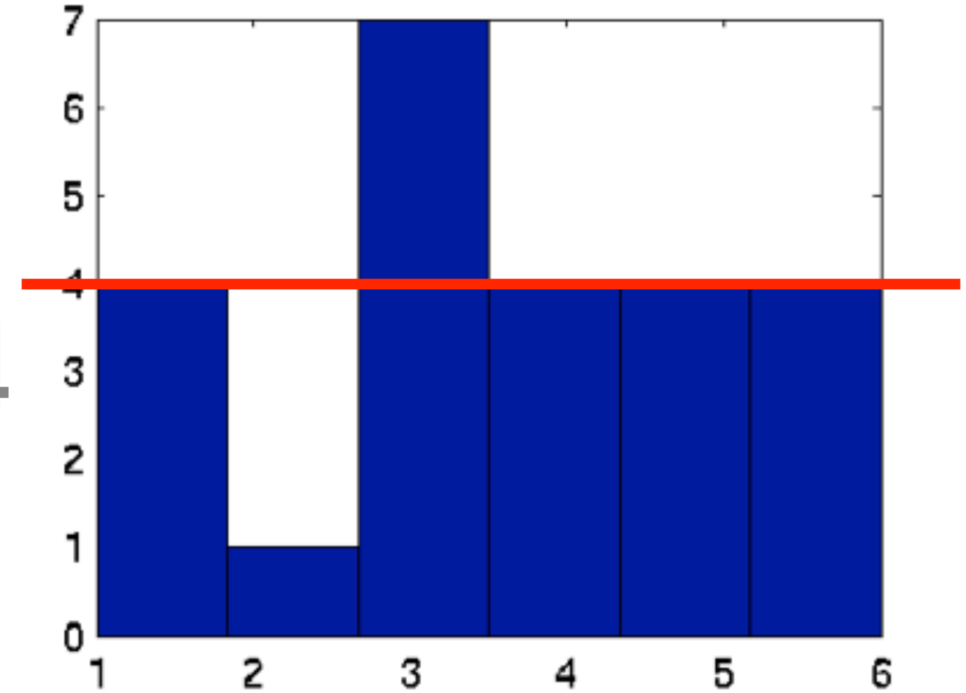

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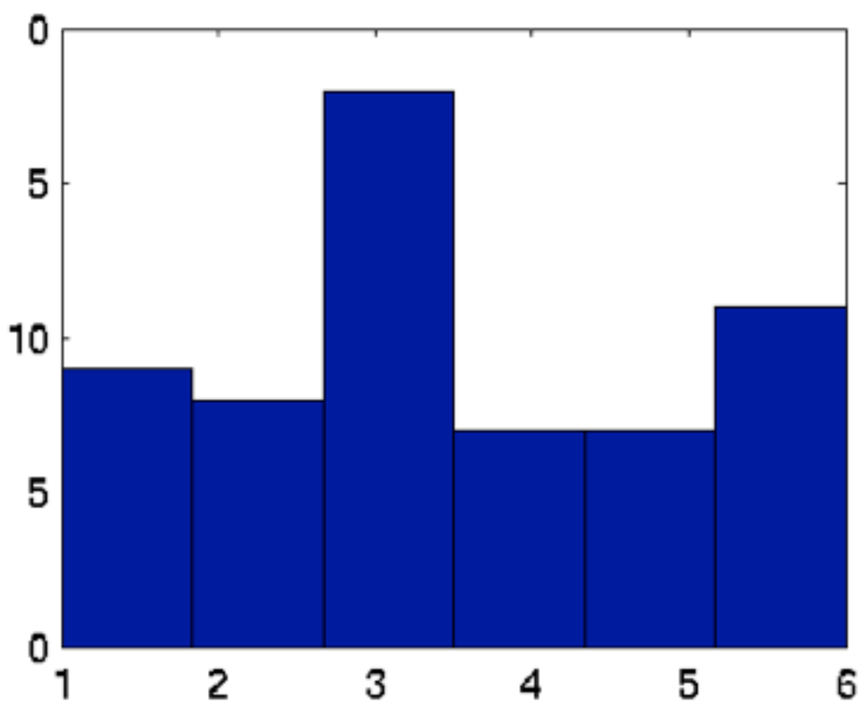

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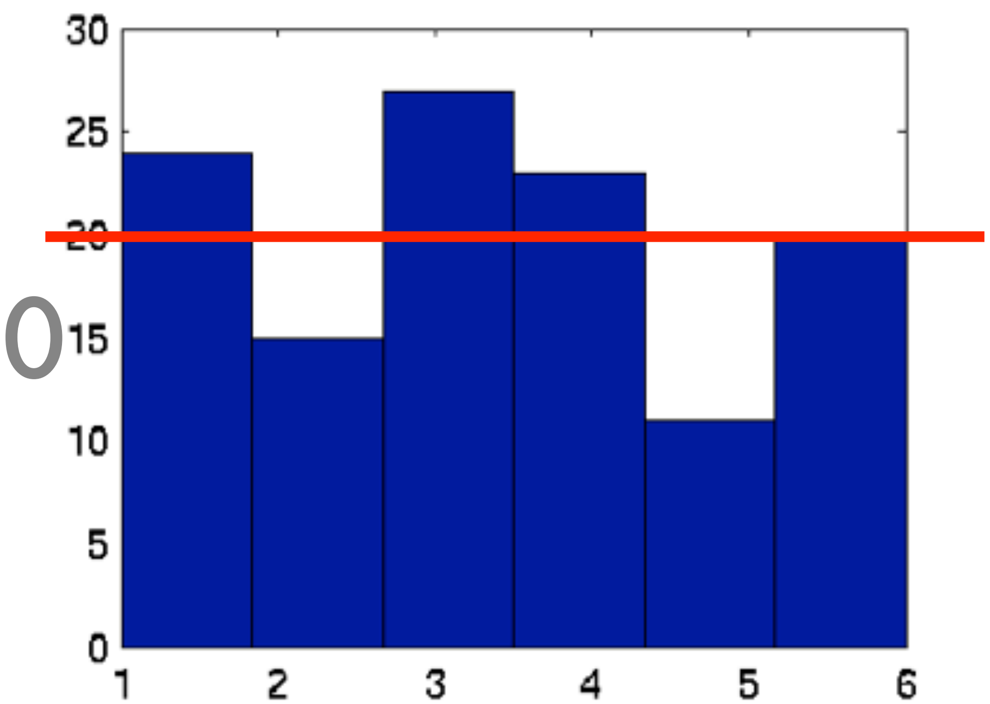
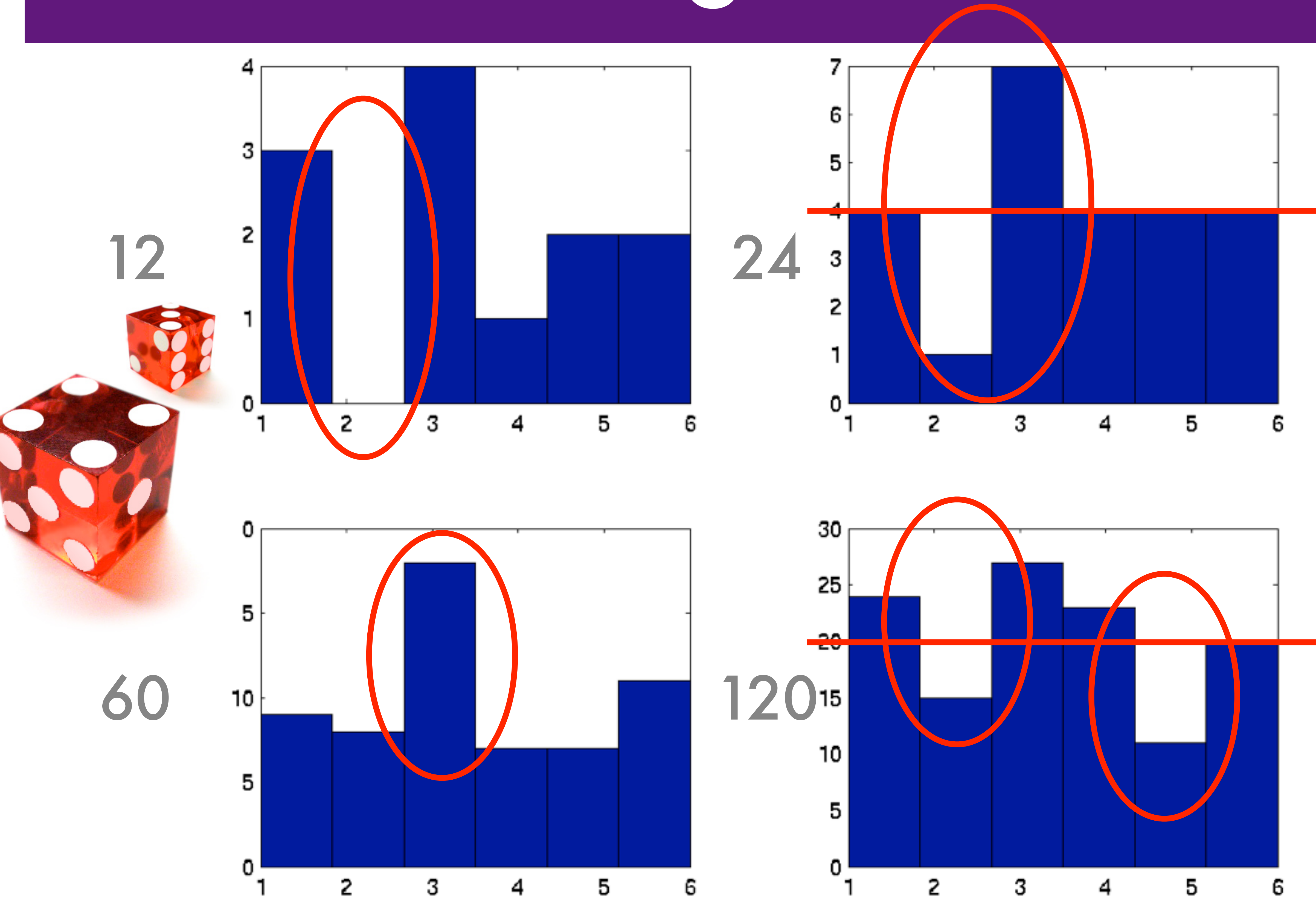


Tossing a Dice

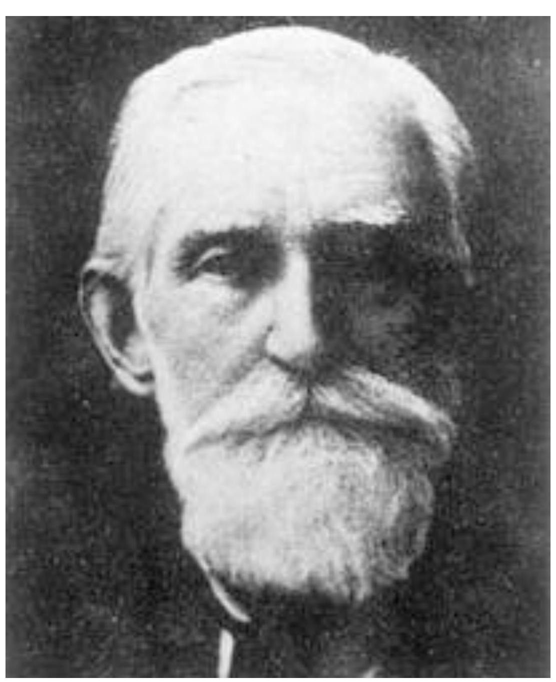


Key Questions

- Do empirical averages converge?
  - Probabilities
  - Means / moments
- Rate of convergence and limit distribution
- Worst case guarantees
- Using prior knowledge

drug testing, semiconductor fabs
computational advertising
user interface design ...

2.2 Tail Bounds



Chebyshev

Chernoff

Hoeffding

Expectations

- Random variable x with probability measure
- Expected value of f(x)

$$\mathbf{E}[f(x)] = \int f(x) dp(x)$$

- Special case - discrete probability mass

$$\Pr\{x = c\} = \mathbf{E}[\{x = c\}] = \int \{x = c\}\, dp(x)$$

(same trick works for intervals)

- Draw x_i identically and independently from p
- Empirical average

$$\mathbf{E}_{\text{emp}}[f(x)] = \frac{1}{n}\sum_{i=1}^{n} f(x_i) \text{ and } \Pr_{\text{emp}}\{x = c\} = \frac{1}{n}\sum_{i=1}^{n}\{x_i = c\}$$

Deviations

- Gambler rolls dice 100 times

$$\hat{P}(X=6) = \frac{1}{n}\sum_{i=1}^{n}\{x_i = 6\}$$

- '6' only occurs 11 times. Fair number is16.7

  IS THE DICE TAINTED?

- Probability of seeing '6' at most 11 times

$$\Pr(X \leq 11) = \sum_{i=0}^{11} p(i) = \sum_{i=0}^{11} \binom{100}{i} \left[\frac{1}{6}\right]^{i} \left[\frac{5}{6}\right]^{100-i} \approx 7.0\%$$

It's probably OK ... can we develop general theory?

Deviations

- Gambler rolls dice 100 times

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IS THE DICE TAINTED?

ad campaign working
new page layout better
drug working

- Probability of seeing '6' at most 11 times

$$\Pr(X \leq 11) = \sum_{i=0}^{11} p(i) = \sum_{i=0}^{11} \binom{100}{i} \left[\frac{1}{6}\right]^i \left[\frac{5}{6}\right]^{100-i} \approx 7.0\%$$

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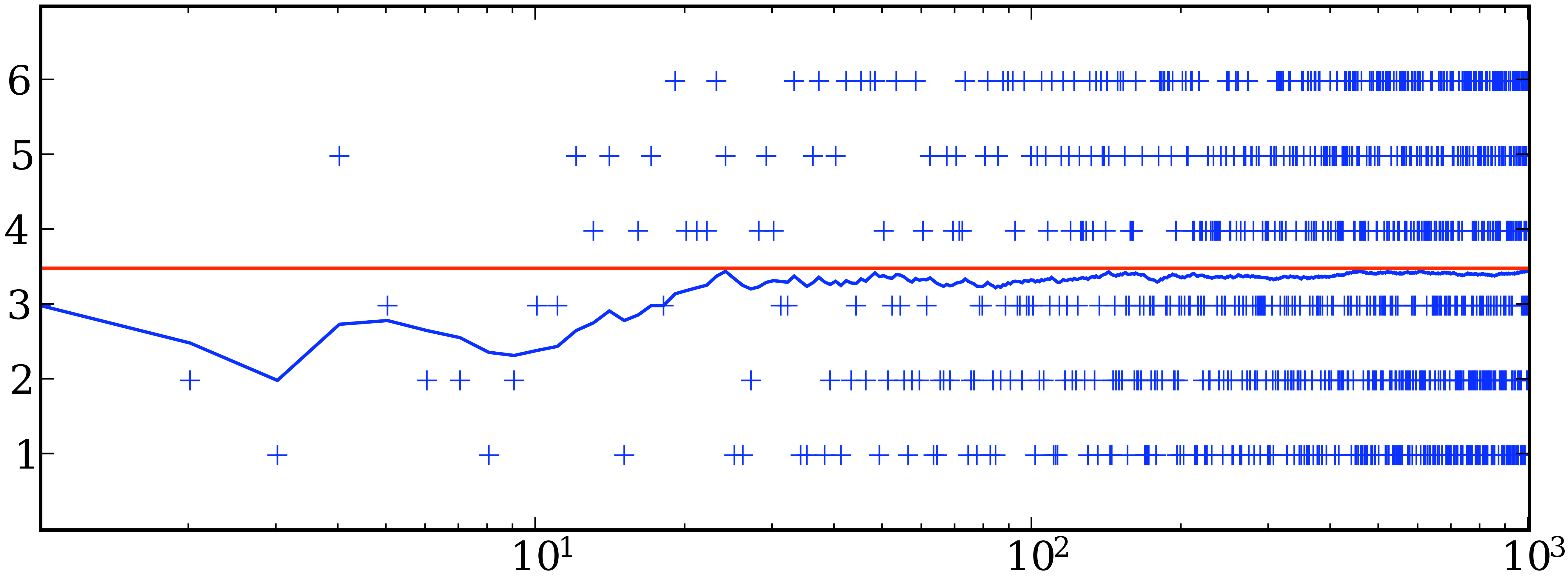
Empirical average for a dice



how quickly does it converge?

Law of Large Numbers

- Random variables x_i with mean $\mu = \mathbf{E}[x_i]$
- Empirical average $\hat{\mu}_n := \frac{1}{n}\sum_{i=1}^{n} x_i$

- **Weak Law of Large Numbers**

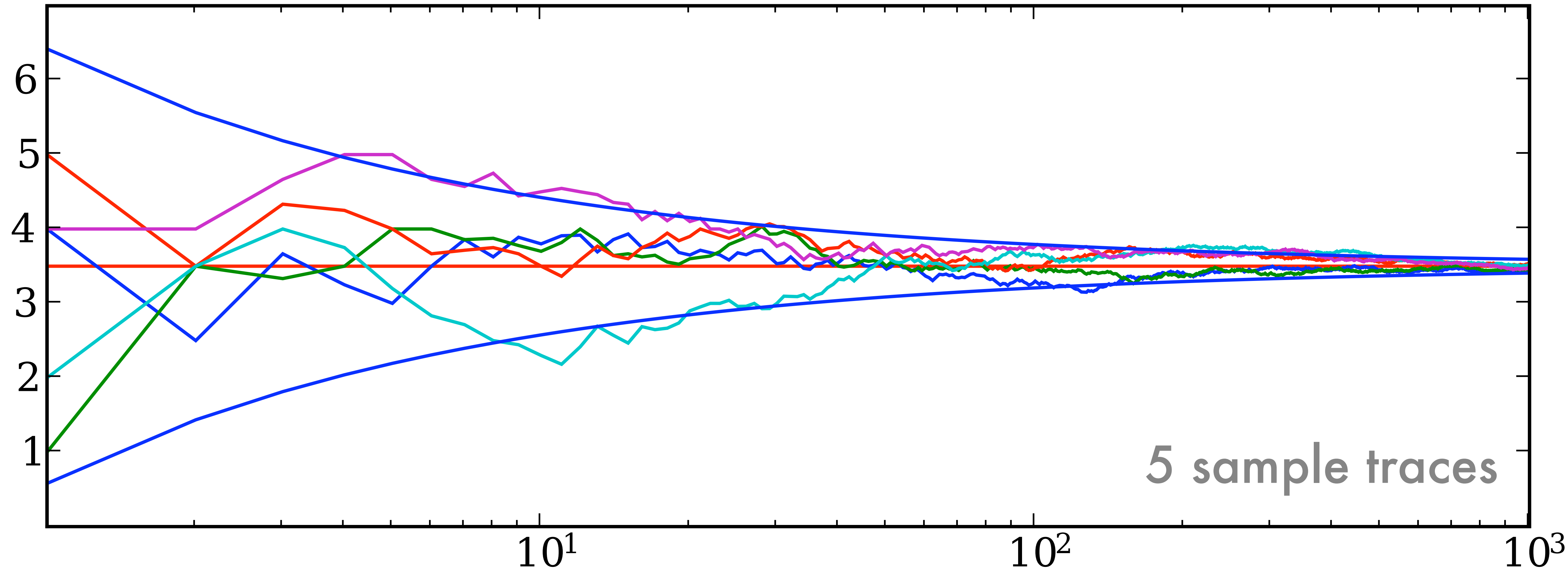
$$\lim_{n\to\infty} \Pr\left(|\hat{\mu}_n - \mu| \leq \epsilon\right) = 1 \text{ for any } \epsilon > 0$$

- **Strong Law of Large Numbers**

$$\Pr\left(\lim_{n\to\infty} \hat{\mu}_n = \mu\right) = 1$$

this means convergence in probability

Empirical average for a dice



- Upper and lower bounds are $\mu \pm \sqrt{\mathrm{Var}(x)/n}$
- This is an example of the central limit theorem

Central Limit Theorem

- Independent random variables x_i with mean μ_i and standard deviation σ_i
- The random variable

$$z_n := \left[\sum_{i=1}^{n} \sigma_i^2\right]^{-\frac{1}{2}} \left[\sum_{i=1}^{n} x_i - \mu_i\right]$$

converges to a Normal Distribution $\mathcal{N}(0, 1)$

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converges to a Normal Distribution $\mathcal{N}(0,1)$

- Special case - IID random variables & average

$$\frac{\sqrt{n}}{\sigma}\left[\frac{1}{n}\sum_{i=1}^{n} x_i - \mu\right] \rightarrow \mathcal{N}(0,1)$$

$O\left(n^{-\frac{1}{2}}\right)$ convergence

Slutsky's Theorem

- Continuous mapping theorem
  - X_i and Y_i sequences of random variables
  - X_i has as its limit the random variable X
  - Y_i has as its limit the constant c
  - g(x,y) is continuous function for all g(x,c)

- $g(X_i, Y_i)$ converges in distribution to g(X,c)

Delta Method

- Random variable X_i convergent to b

$$a_n^{-2}(X_n - b) \to \mathcal{N}(0, \Sigma) \text{ with } a_n^2 \to 0 \text{ for } n \to \infty$$

- g is a continuously differentiable function for b
- Then $g(X_i)$ inherits convergence properties

$$a_n^{-2}\left(g(X_n) - g(b)\right) \to \mathcal{N}(0, [\nabla_x g(b)]\Sigma[\nabla_x g(b)]^\top)$$

- Proof: use Taylor expansion for $g(X_n)$ - g(b)

$$a_n^{-2}\left[g(X_n) - g(b)\right] = [\nabla_x g(\xi_n)]^\top a_n^{-2}(X_n - b)$$

  - $g(\xi_n)$ is on line segment $[X_n, b]$
  - By Slutsky's theorem it converges to g(b)
  - Hence $g(X_i)$ is asymptotically normal

Tools for the proof

Fourier Transform

- Fourier transform relations

$$F[f](\omega) := (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^n} f(x) \exp(-i \langle \omega, x \rangle) dx$$

$$F^{-1}[g](x) := (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^n} g(\omega) \exp(i \langle \omega, x \rangle) d\omega.$$

- Useful identities
  - Identity

$$F^{-1} \circ F = F \circ F^{-1} = \mathrm{Id}$$

  - Derivative

$$F[\partial_x f] = -i\omega F[f]$$

  - Convolution (also holds for inverse transform)

$$F[f \circ g] = (2\pi)^{\frac{d}{2}} F[f] \cdot F[g]$$

The Characteristic Function Method

- Characteristic function

$$\phi_X(\omega) := F^{-1}[p(x)] = \int \exp(i \langle \omega, x \rangle) dp(x)$$

- For X and Y independent we have
  - Joint distribution is convolution

$$p_{X+Y}(z) = \int p_X(z-y) p_Y(y) dy = p_X \circ p_Y$$

  - Characteristic function is product

$$\phi_{X+Y}(\omega) = \phi_X(\omega) \cdot \phi_Y(\omega)$$

  - Proof - plug in definition of Fourier transform
- Characteristic function is unique

Proof - Weak law of large numbers

- Require that expectation exists
- Taylor expansion of exponential

$$\exp(iwx) = 1 + i\langle w, x\rangle + o(|w|)$$
$$\text{and hence } \phi_X(\omega) = 1 + iw\mathbf{E}_X[x] + o(|w|).$$

(need to assume that we can bound the tail)

- Average of random variables

$$\phi_{\hat{\mu}_m}(\omega) = \left(1 + \frac{i}{m} w\mu + o(m^{-1}|w|)\right)^m$$

convolution

vanishing higher order terms

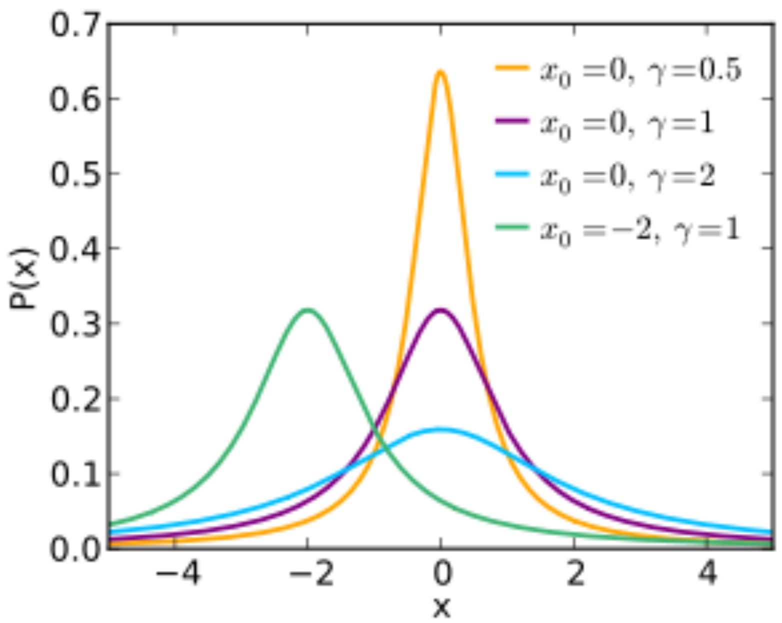
- Limit is constant distribution

$$\phi_{\hat{\mu}_m}(\omega) \to \exp i\omega\mu = 1 + i\omega\mu + \ldots$$

mean

Warning

- Moments may not always exist
  - Cauchy distribution



$$p(x) = \frac{1}{\pi}\frac{1}{1+x^2}$$

  - For the mean to exist the following integral would have to converge

$$\int |x| dp(x) \geq \frac{2}{\pi}\int_1^\infty \frac{x}{1+x^2}dx \geq \frac{1}{\pi}\int_1^\infty \frac{1}{x}dx = \infty$$

Proof - Central limit theorem

- Require that second order moment exists (we assume they're all identical WLOG)
- Characteristic function

$$\exp(iwx) = 1 + iwx - \frac{1}{2}w^2x^2 + o(|w|^2)$$

$$\text{and hence } \phi_X(\omega) = 1 + iw\mathbf{E}_X[x] - \frac{1}{2}w^2\text{var}_X[x] + o(|w|^2)$$

- Subtract out mean (centering) $z_n := \left[\sum_{i=1}^n \sigma_i^2\right]^{-\frac{1}{2}} \left[\sum_{i=1}^n x_i - \mu_i\right]$

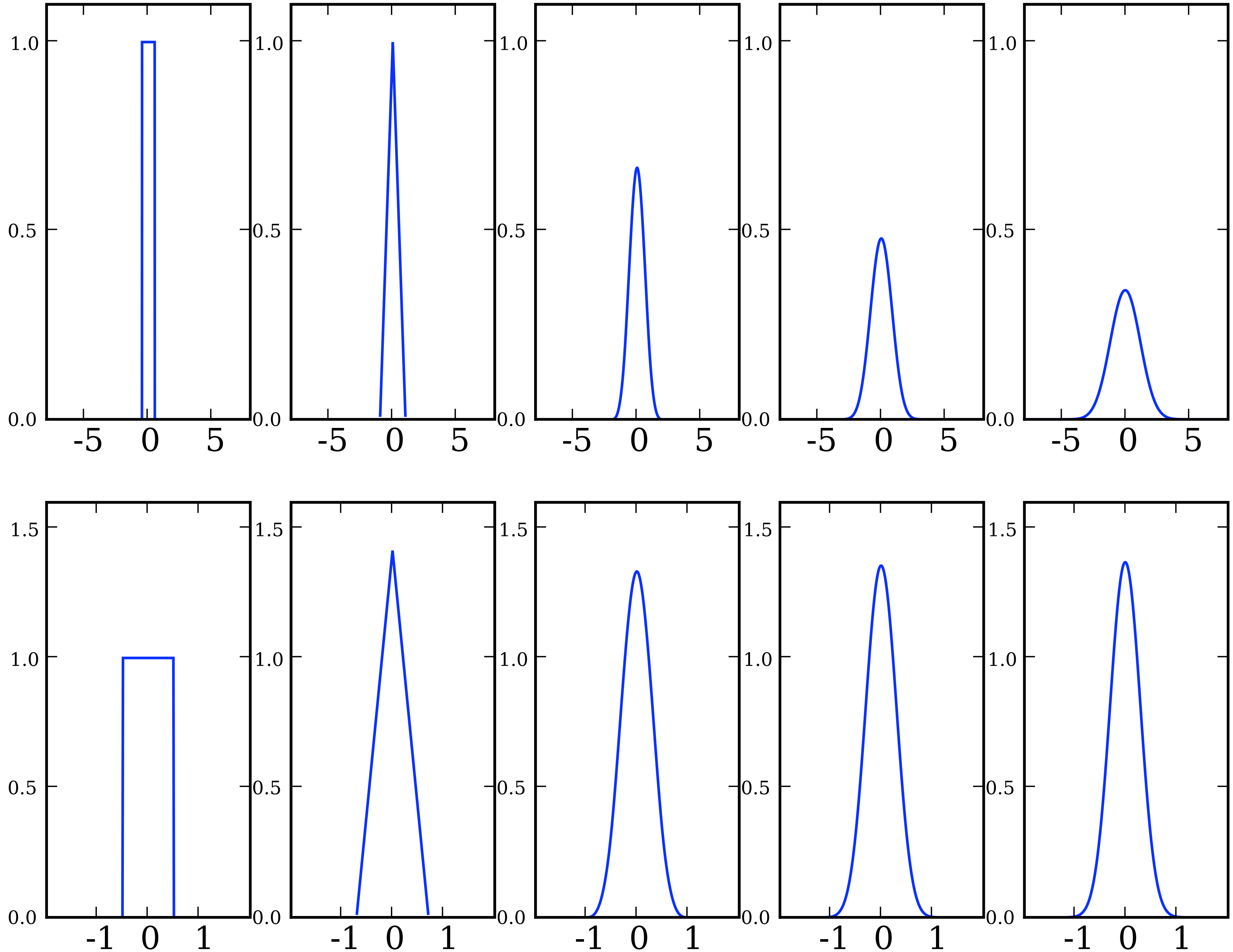
$$\phi_{Z_m}(\omega) = \left(1 - \frac{1}{2m}w^2 + o(m^{-1}|w|^2)\right)^m \to \exp\left(-\frac{1}{2}w^2\right) \text{ for } m \to \infty$$

This is the FT of a Normal Distribution

Central Limit Theorem in Practice

unscaled

scaled



Finite sample tail bounds

Simple tail bounds

- Gauss Markov inequality

  Random variable X with mean μ

  $$\Pr(X \geq \epsilon) \leq \mu/\epsilon$$

  Proof - decompose expectation

  $$\Pr(X \geq \epsilon) = \int_\epsilon^\infty dp(x) \leq \int_\epsilon^\infty \frac{x}{\epsilon} dp(x) \leq \epsilon^{-1} \int_0^\infty x dp(x) = \frac{\mu}{\epsilon}.$$

- Chebyshev inequality

  Random variable X with mean μ and variance σ^2

  $$\Pr(|\hat{\mu}_m - \mu\| > \epsilon) \leq \sigma^2 m^{-1} \epsilon^{-2} \text{ or equivalently } \epsilon \leq \sigma/\sqrt{m\delta}$$

  Proof - applying Gauss-Markov to $Y = (X - \mu)^2$ with confidence ε^2 yields the result.

Scaling behavior

- Gauss-Markov

$$\epsilon \leq \frac{\mu}{\delta}$$

  Scales properly in μ but expensive in δ

- Chebyshev

$$\epsilon \leq \frac{\sigma}{\sqrt{m\delta}}$$

  Proper scaling in σ but still bad in δ

Can we get logarithmic scaling in δ?

Chernoff bound

- KL-divergence variant of Chernoff bound

$$K(p,q) = p\log\frac{p}{q} + (1-p)\log\frac{1-p}{1-q}$$

- n independent tosses from biased coin with p

$$\Pr\left\{\sum_i x_i \geq nq\right\} \leq \exp\left(-nK(q,p)\right) \leq \exp\left(-2n(p-q)^2\right)$$

Pinsker's inequality

- Proof w.l.o.g. $q > p$ and set $k \geq qn$

$$\frac{\Pr\left\{\sum_i x_i = k|q\right\}}{\Pr\left\{\sum_i x_i = k|p\right\}} = \frac{q^k(1-q)^{n-k}}{p^k(1-p)^{n-k}} \geq \frac{q^{qn}(1-q)^{n-qn}}{p^{qn}(1-p)^{n-qn}} = \exp\left(nK(q,p)\right)$$

$$\sum_{k\geq nq}\Pr\left\{\sum_i x_i = k|p\right\} \leq \sum_{k\geq nq}\Pr\left\{\sum_i x_i = k|q\right\}\exp(-nK(q,p)) \leq \exp(-nK(q,p))$$

McDiarmid Inequality

- Independent random variables X_i
- Function $f : \mathcal{X}^m \to \mathbb{R}$
- Deviation from expected value

  $$\Pr\left(|f(x_1, \ldots, x_m) - \mathbf{E}_{X_1, \ldots, X_m}[f(x_1, \ldots, x_m)]| > \epsilon\right) \leq 2 \exp\left(-2\epsilon^2 C^{-2}\right)$$

  Here C is given by $C^2 = \sum_{i=1}^{m} c_i^2$ where

  $$|f(x_1, \ldots, x_i, \ldots, x_m) - f(x_1, \ldots, x_i', \ldots, x_m)| \leq c_i$$

- Hoeffding's theorem

  f is average and X_i have bounded range c

  $$\Pr\left(|\hat{\mu}_m - \mu| > \epsilon\right) \leq 2 \exp\left(-\frac{2m\epsilon^2}{c^2}\right).$$

Scaling behavior

- Hoeffding

$$\delta := \Pr\left(|\hat{\mu}_m - \mu| > \epsilon\right) \leq 2\exp\left(-\frac{2m\epsilon^2}{c^2}\right)$$

$$\implies \log\delta/2 \leq -\frac{2m\epsilon^2}{c^2}$$

$$\implies \epsilon \leq c\sqrt{\frac{\log 2 - \log\delta}{2m}}$$

This helps when we need to combine several tail bounds since we only pay logarithmically in terms of their combination.

More tail bounds

- Higher order moments
  - Bernstein inequality (needs variance bound)

$$\Pr\left(\mu_m - \mu \geq \epsilon\right) \leq \exp\left(-\frac{t^2/2}{\sum_i \mathbf{E}[X_i^2] + Mt/3}\right)$$

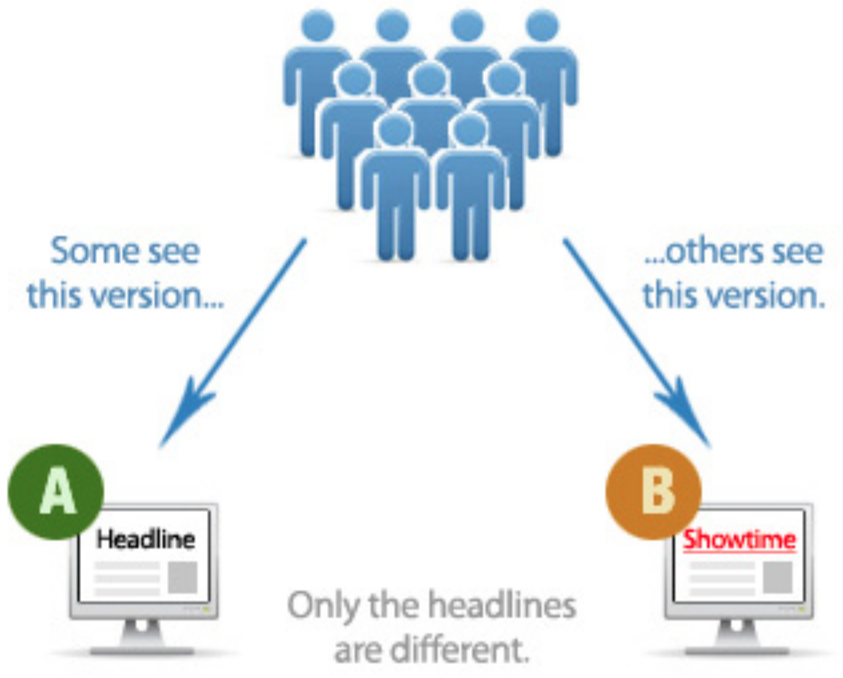
    here M upper-bounds the random variables X_i
  - Proof via Gauss-Markov inequality applied to exponential sums (hence exp. inequality)
  - See also Azuma, Bennett, Chernoff, ...
- Absolute / relative error bounds
- Bounds for (weakly) dependent random variables

Tail bounds in practice

A/B testing

- Two possible webpage layouts
- Which layout is better?

- Experiment
  - Half of the users see A
  - The other half sees design B



- How many trials do we need to decide which page attracts more clicks?

Assume that the probabilities are p(A) = 0.1 and p(B) = 0.11 respectively and that p(A) is known

Chebyshev Inequality

- Need to bound for a deviation of 0.01
- Mean is p(B) = 0.11 (we don't know this yet)
- Want failure probability of 5%

- If we have no prior knowledge, we can only bound the variance by $\sigma^2 = 0.25$

$$m \leq \frac{\sigma^2}{\epsilon^2 \delta} = \frac{0.25}{0.01^2 \cdot 0.05} = 50,000$$

- If we know that the click probability is at most 0.15 we can bound the variance at 0.15 * 0.85 = 0.1275. This requires at most 25,500 users.

Hoeffding's bound

- Random variable has bounded range [0, 1] (click or no click), hence c=1
- Solve Hoeffding's inequality for m

$$m \leq -\frac{c^2 \log \delta/2}{2\epsilon^2} = -\frac{1 \cdot \log 0.025}{2 \cdot 0.01^2} < 18,445$$

This is slightly better than Chebyshev.

Normal Approximation (Central Limit Theorem)

- Use asymptotic normality
- Gaussian interval containing 0.95 probability

$$\frac{1}{2\pi\sigma^2}\int_{\mu-\epsilon}^{\mu+\epsilon} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = 0.95$$

  is given by ε = 2.96σ.
- Use variance bound of 0.1275 (see Chebyshev)

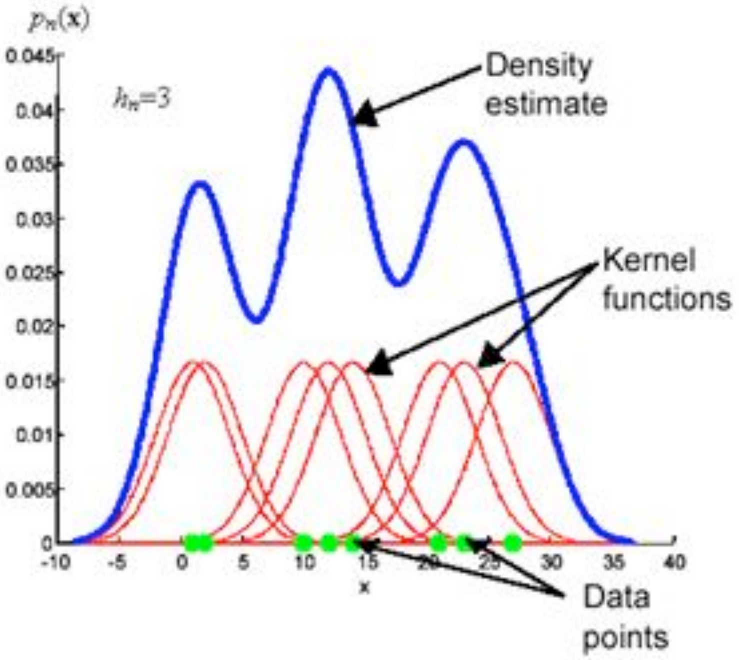
$$m \leq \frac{2.96^2\sigma^2}{\epsilon^2} = \frac{2.96^2 \cdot 0.1275}{0.01^2} \leq 11,172$$

  Same rate as Hoeffding bound!
  Better bounds by bounding the variance.

Beyond

- Many different layouts?
- Combinatorial strategy to generate them (aka the Thai Restaurant process)
- What if it depends on the user / time of day
- Stateful user (e.g. query keywords in search)
- What if we have a good prior of the response (rather than variance bound)?

- Explore/exploit/reinforcement learning/control (more details at the end of this class)



2.3 Kernel Density Estimation

Parzen

Density Estimation

- For discrete bins (e.g. male/female; English/French/German/Spanish/Chinese) we get good uniform convergence:
  - Applying the union bound and Hoeffding

$$\Pr\left(\sup_{a\in A}|\hat{p}(a)-p(a)|\geq\epsilon\right)\leq\sum_{a\in A}\Pr\left(|\hat{p}(a)-p(a)|\geq\epsilon\right)$$

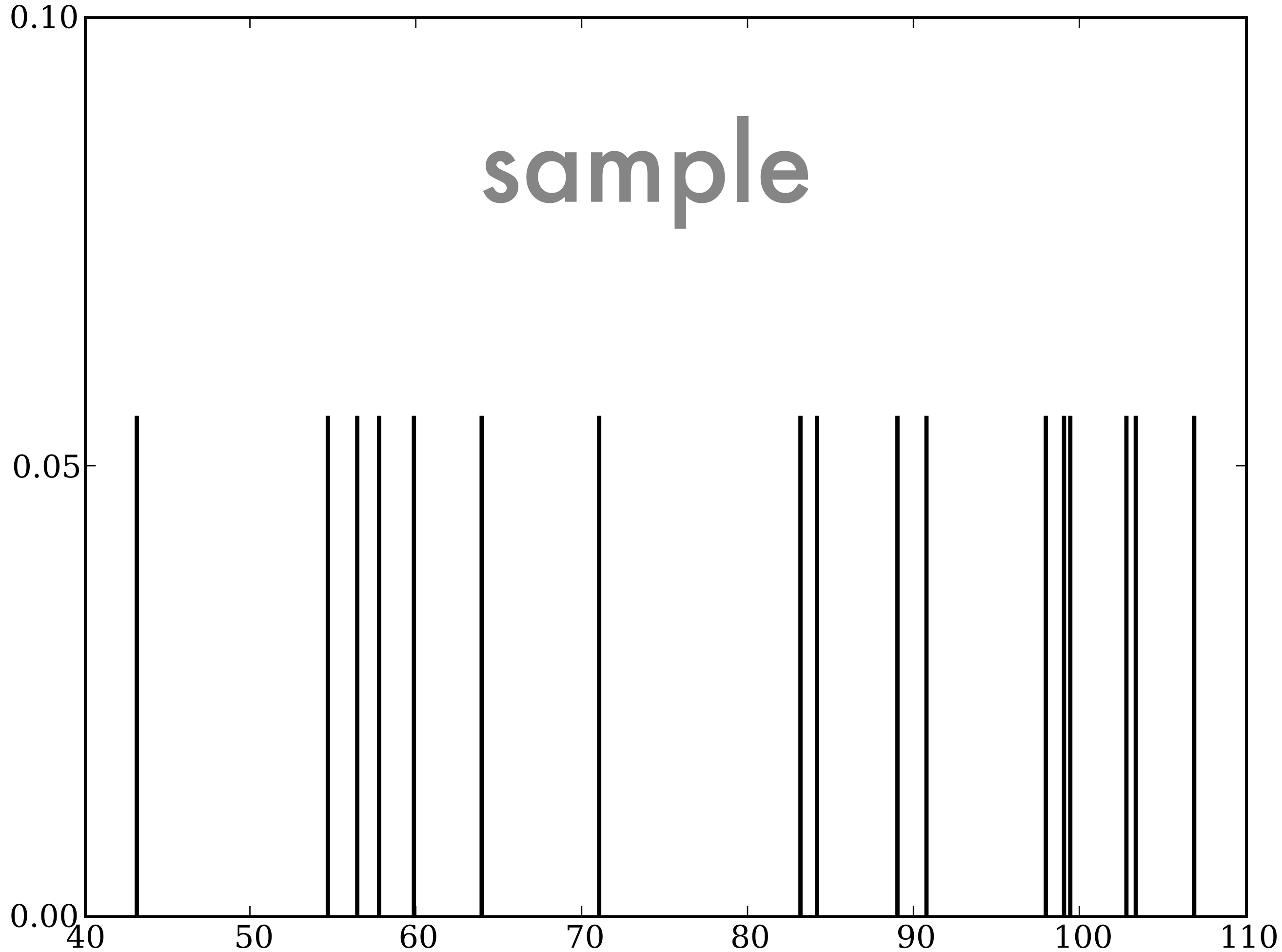
$$\leq 2|A|\exp\left(-2m\epsilon^2\right)$$

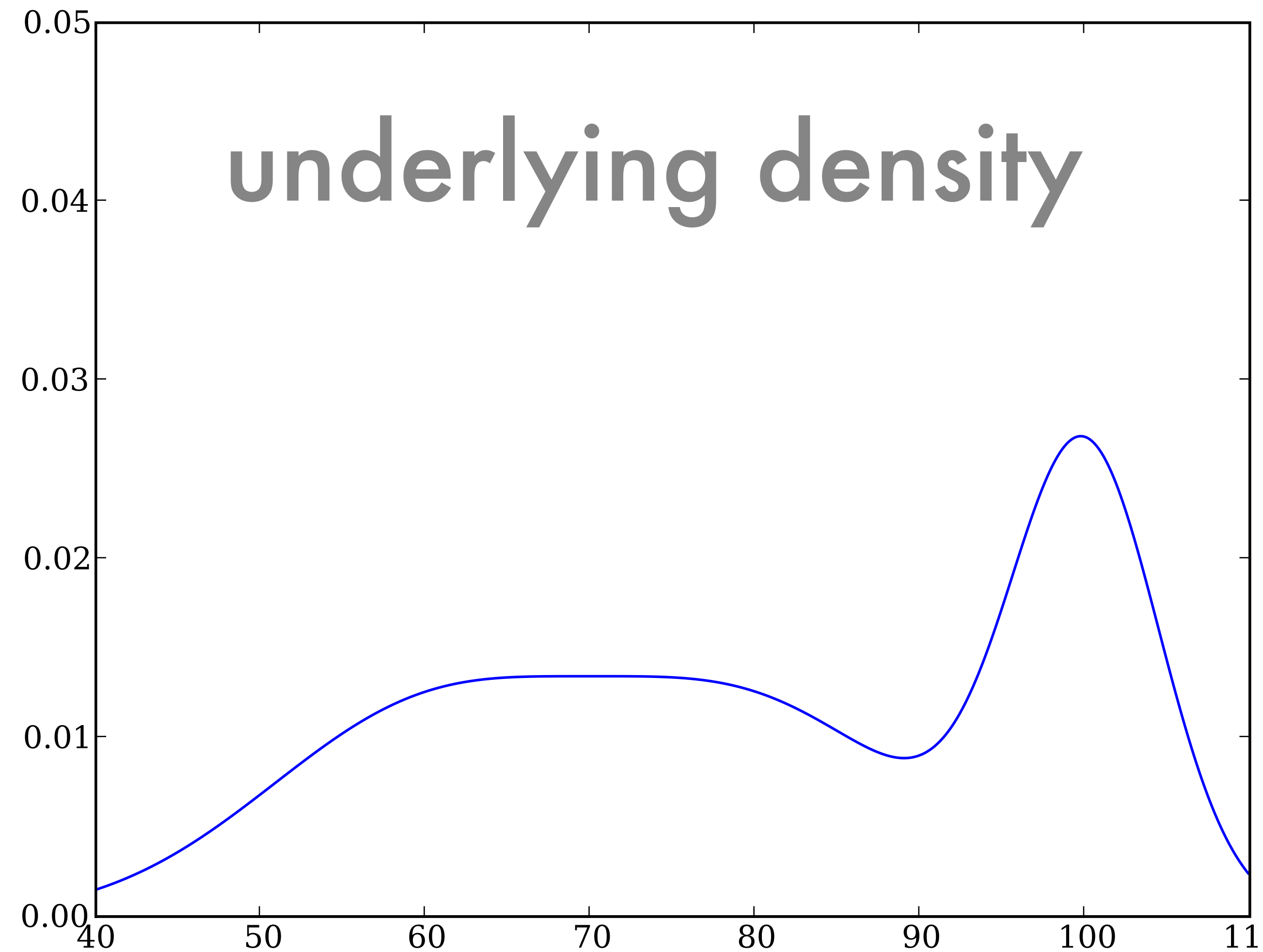
  - Solving for error probability

good news

$$\frac{\delta}{2|A|}\leq\exp(-m\epsilon^2)\implies\epsilon\leq\sqrt{\frac{\log 2|A|-\log\delta}{2m}}$$

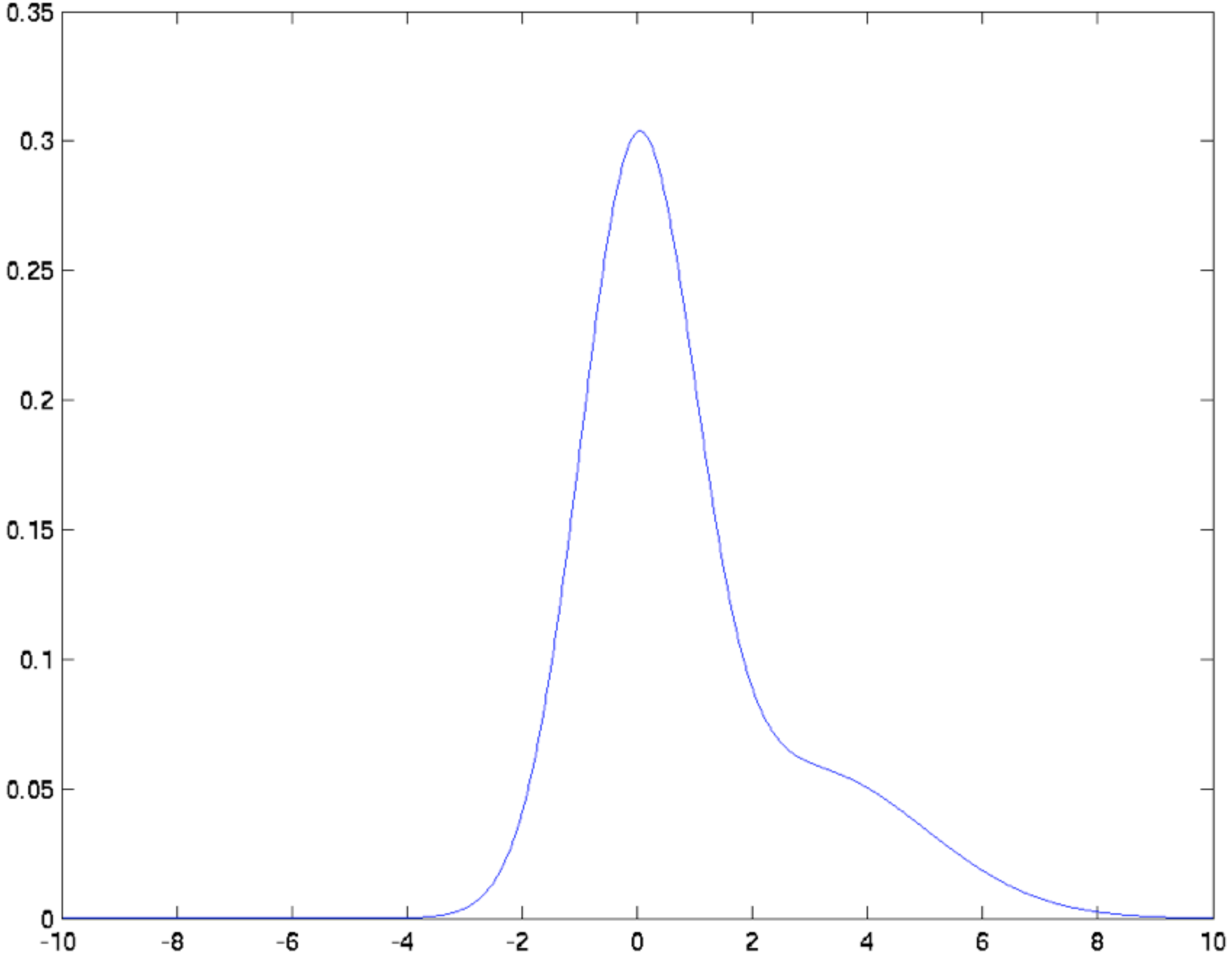
Density Estimation



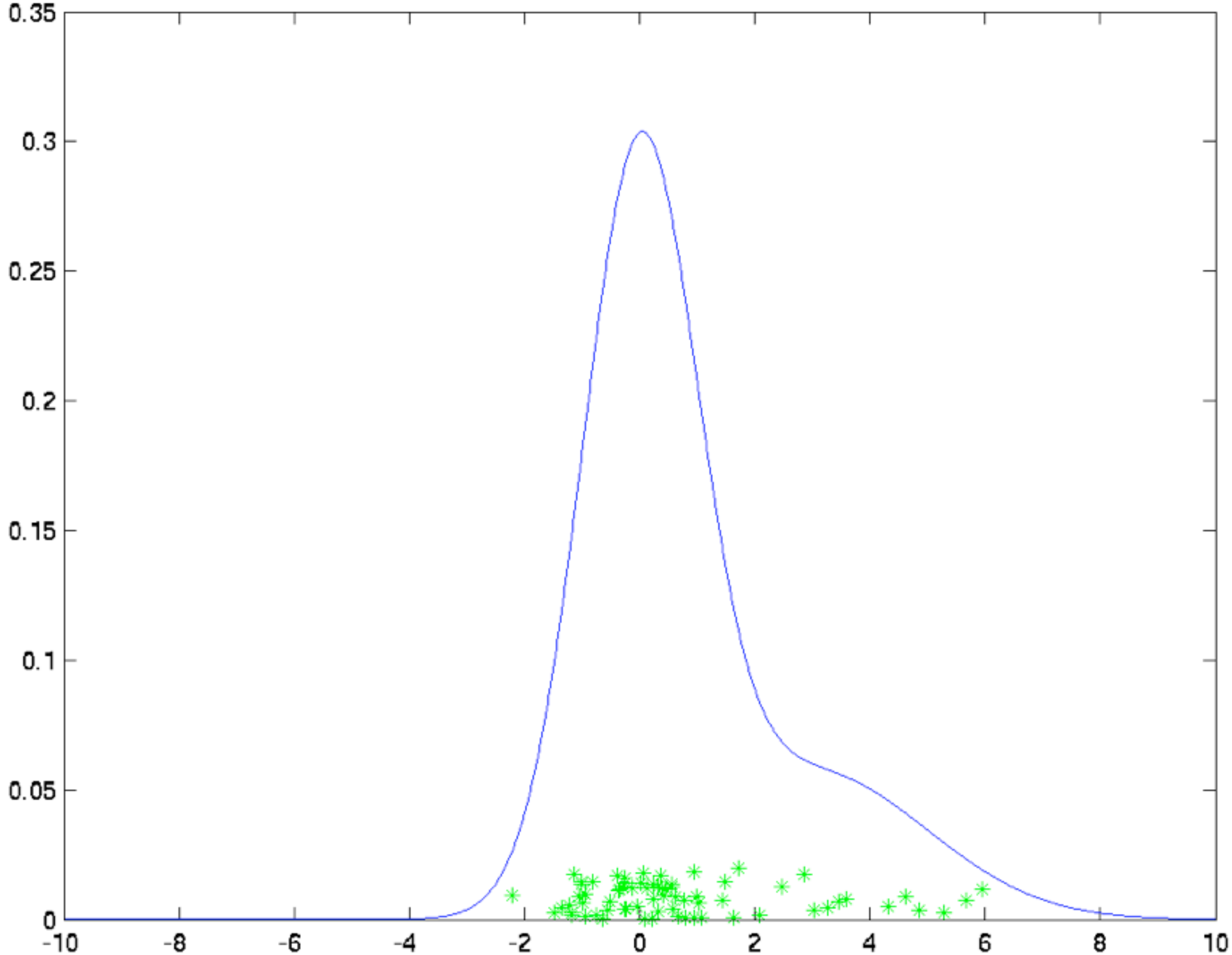


- Continuous domain = infinite number of bins
- Curse of dimensionality
  - 10 bins on [0, 1] is probably good
  - 10^{10} bins on $[0, 1]^{10}$ requires high accuracy in estimate: probability mass per cell also decreases by 10^{10}.

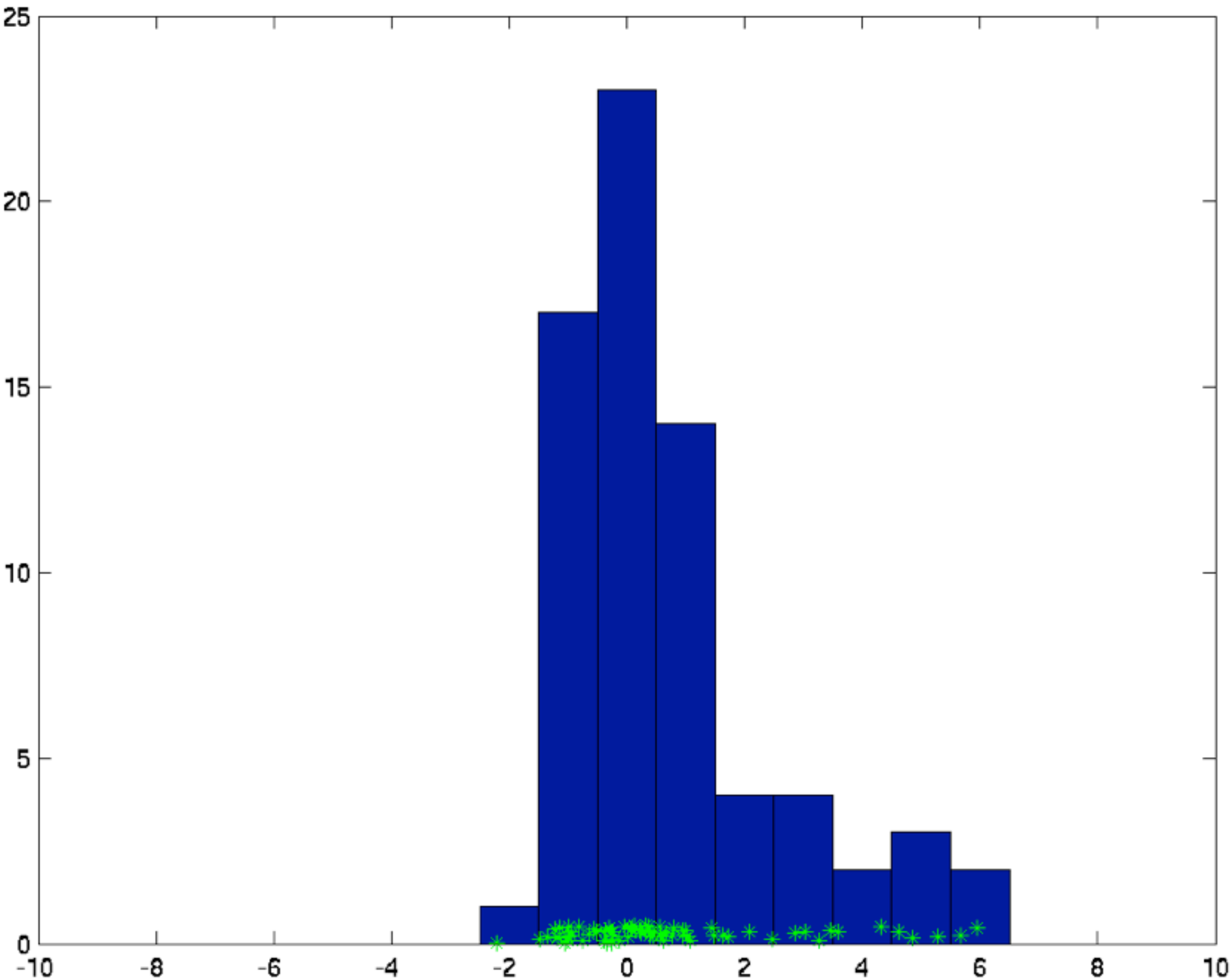
Bin Counting



Bin Counting



Bin Counting



Parzen Windows

- Naive approach
  Use empirical density (delta distributions)

$$p_{\text{emp}}(x) = \frac{1}{m} \sum_{i=1}^{m} \delta_{x_i}(x)$$

- This breaks if we see slightly different instances
- Kernel density estimate
  Smear out empirical density with a nonnegative smoothing kernel $k_x(x')$ satisfying

$$\int_{\mathcal{X}} k_x(x') dx' = 1 \text{ for all } x$$

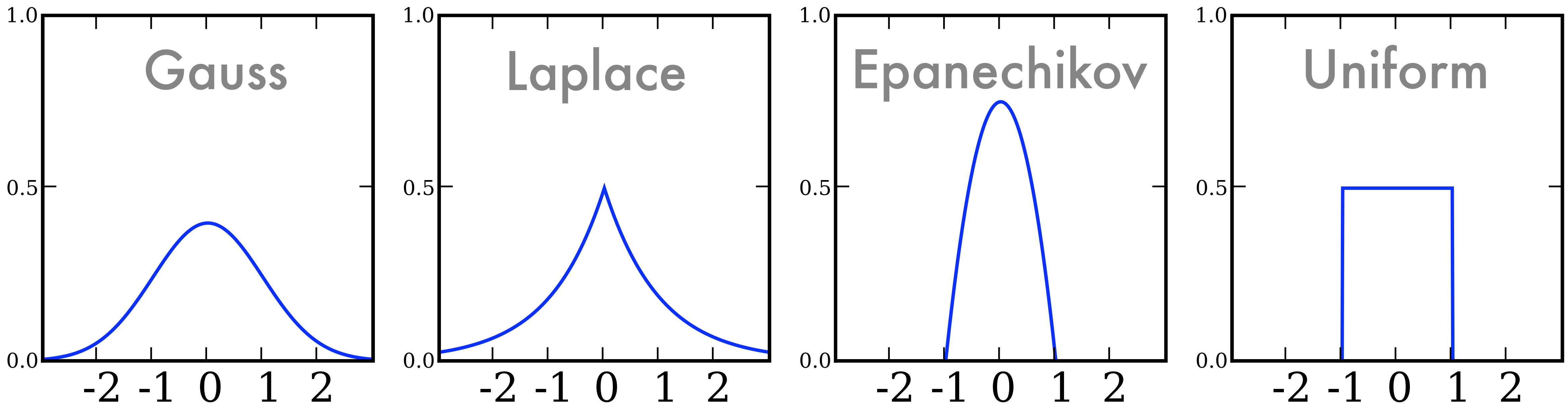
Parzen Windows

- Density estimate

$$p_{\text{emp}}(x) = \frac{1}{m}\sum_{i=1}^{m} \delta_{x_i}(x)$$

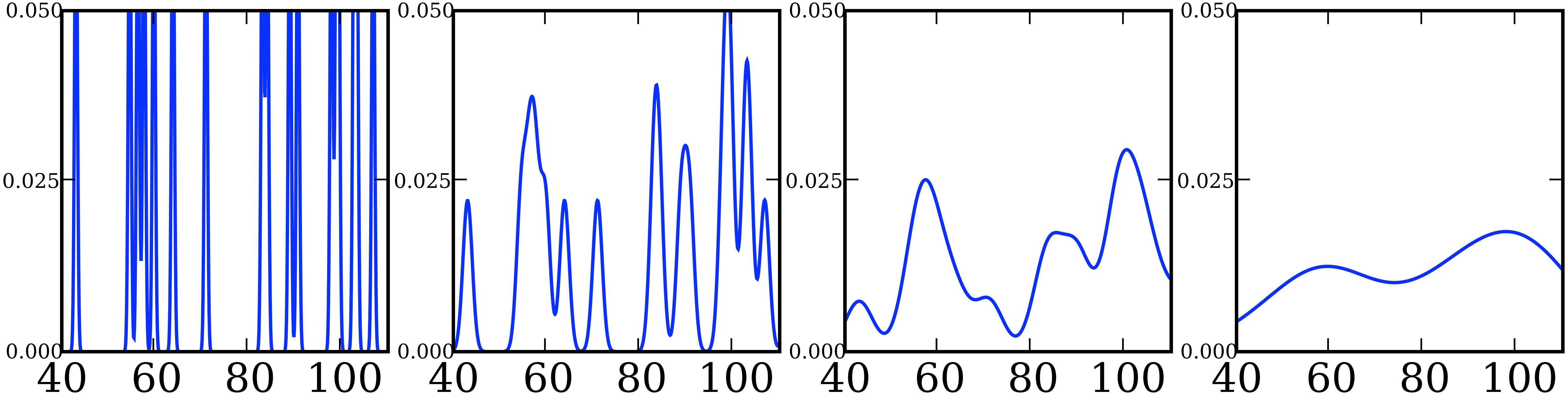
$$\hat{p}(x) = \frac{1}{m}\sum_{i=1}^{m} k_{x_i}(x)$$

- Smoothing kernels

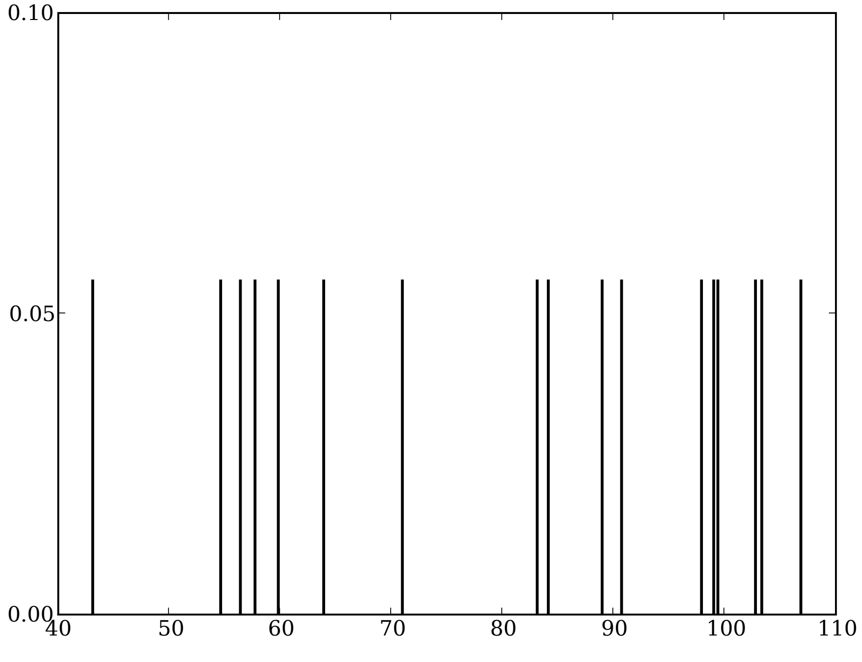


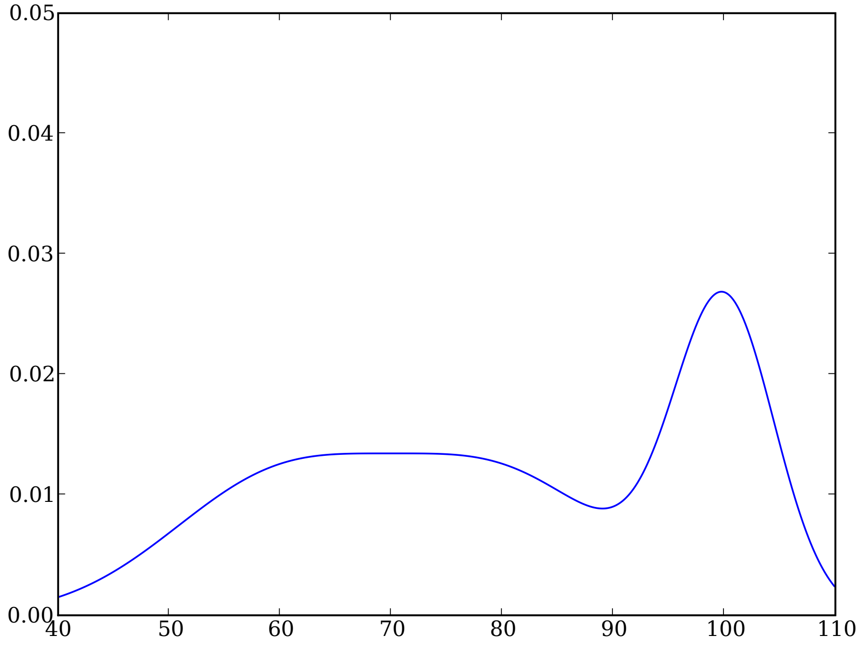
$(2\pi)^{-\frac{1}{2}} e^{-\frac{1}{2}x^2}$ $\frac{1}{2}e^{-|x|}$ $\frac{3}{4}\max(0, 1-x^2)$ $\frac{1}{2}\chi_{[-1,1]}(x)$

Size matters

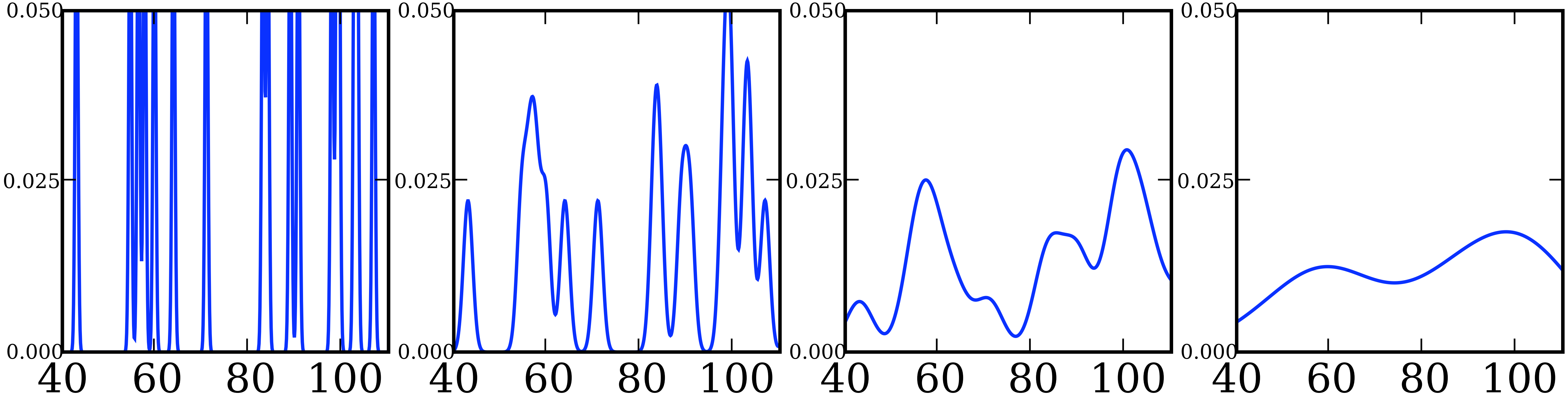


0.3 1 3 10



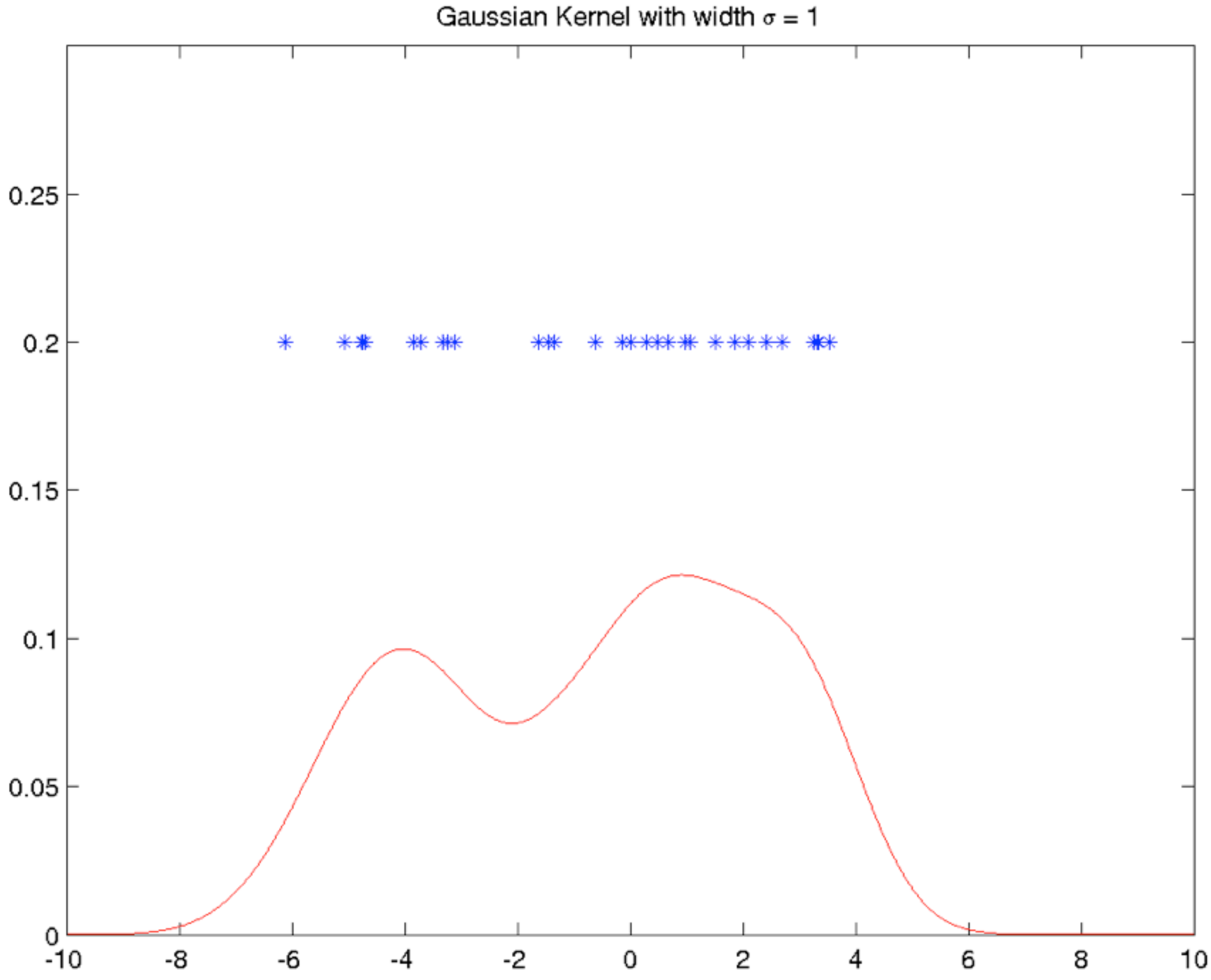


Size matters

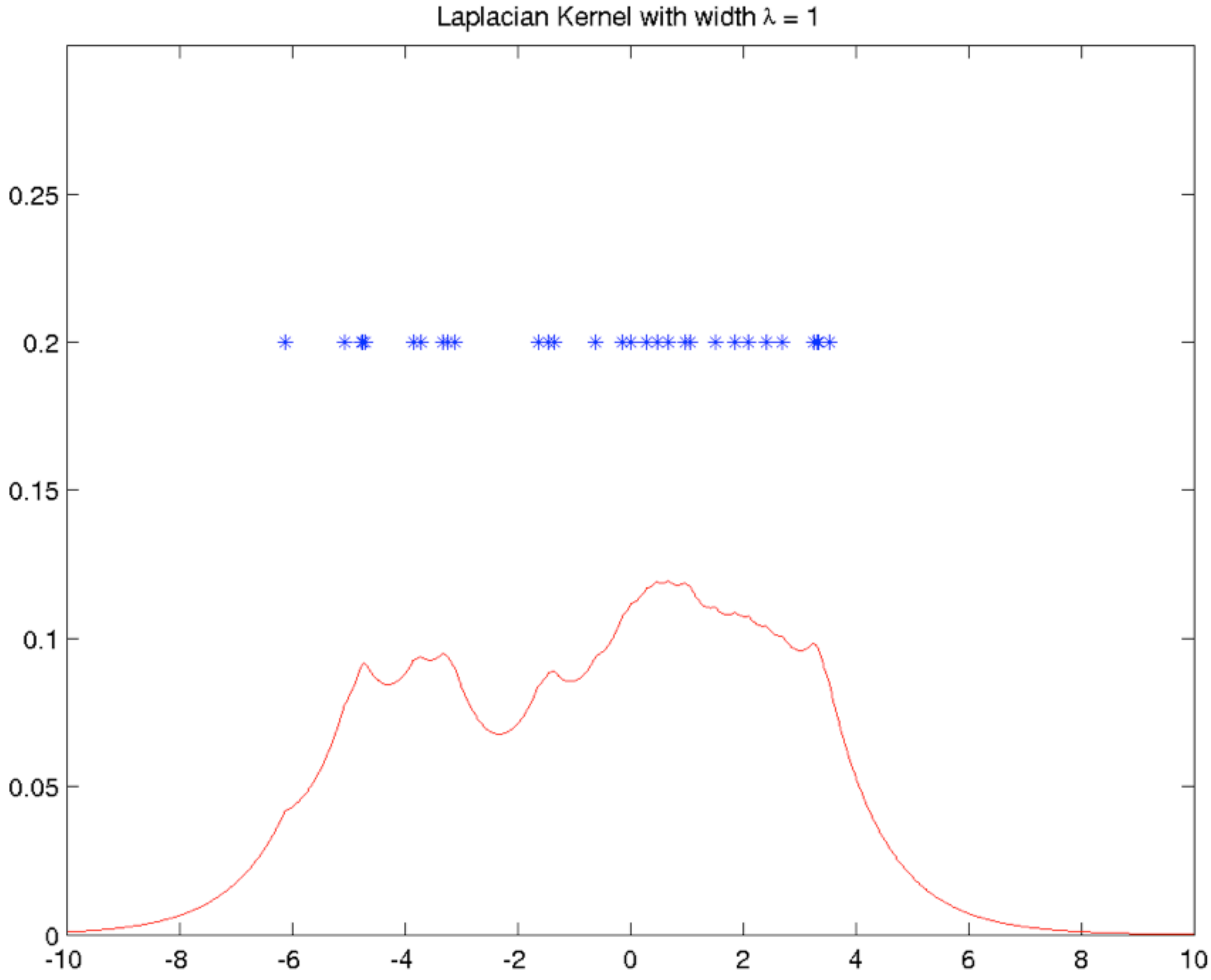


- Kernel width $$k_{x_i}(x) = r^{-d} h\left(\frac{x - x_i}{r}\right)$$
  - Too narrow overfits
  - Too wide smoothes with constant distribution
- How to choose?

Smoothing

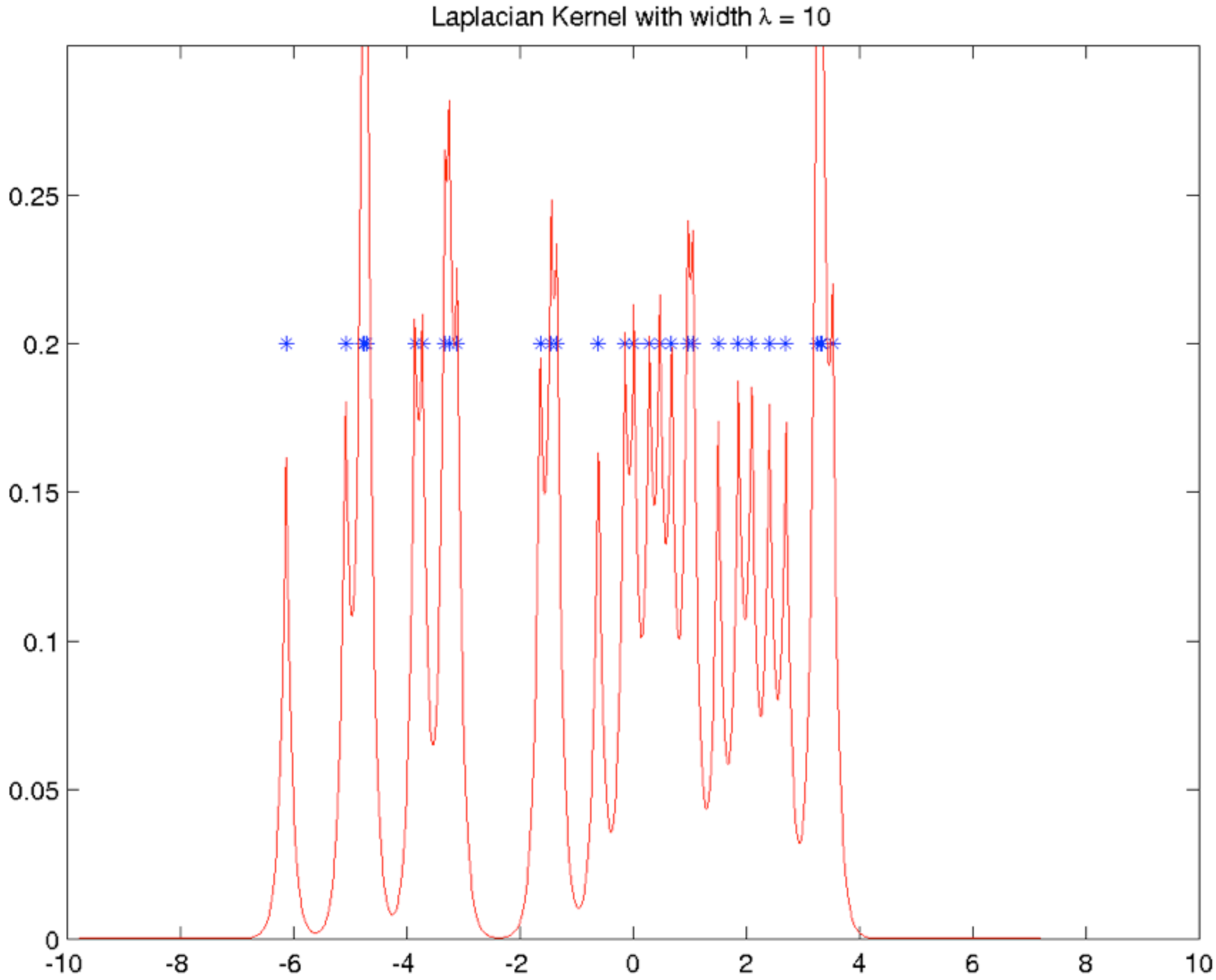

Gaussian Kernel with width σ = 1
0.25
0.2
0.15
0.1
0.05
0
-10
-8
-6
-4
-2
0
2
4
6
8
10

Smoothing



Laplacian Kernel with width λ = 1
0.25
0.2
0.15
0.1
0.05
0
-10
-8
-6
-4
-2
0
2
4
6
8
10

Smoothing



Laplacian Kernel with width λ = 10
0.25
0.2
0.15
0.1
0.05
0
-10
-8
-6
-4
-2
0
2
4
6
8
10

Capacity Control

Capacity control

- Need automatic mechanism to select scale
- Overfitting
  - Maximum likelihood will lead to r=0 (smoothing kernels peak at instances)
  - This is (typically) a set of measure 0.
- Validation set
  Set aside data just for calibrating r
- Leave-one-out estimation
  Estimate likelihood using all but one instance
- Alternatives: use a prior on r; convergence analysis

Capacity Control

- **Validation set**

$$\log \hat{p}(X') = \sum_{x' \in X'} \log \hat{p}(x')$$

$$= \sum_{x' \in X'} \log \sum_{x \in X} k\left(\frac{x - x'}{r}\right) - |X'| \left[d \log r + \log |X|\right]$$

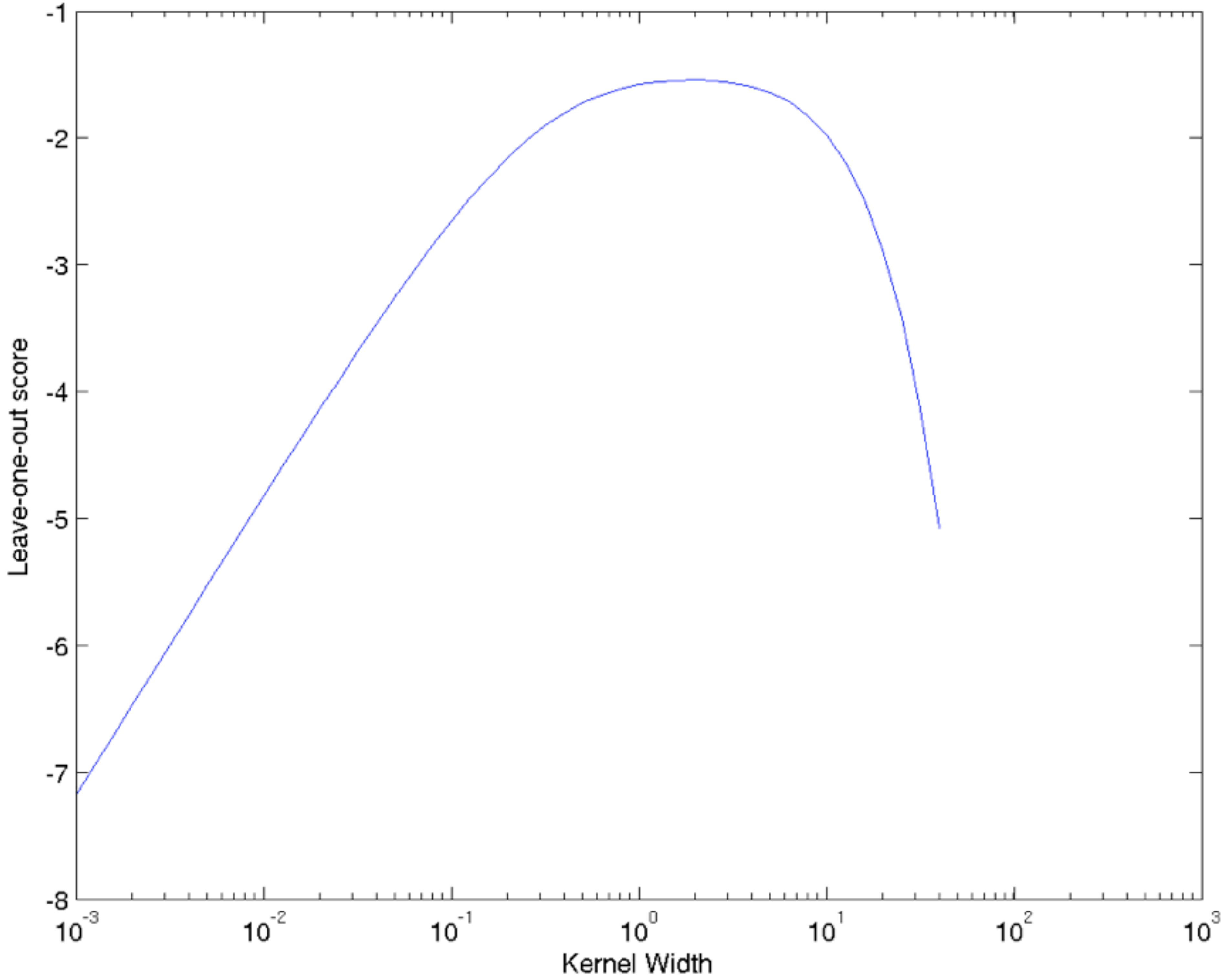
- **Leave-one-out crossvalidation**

$$\hat{p}_{X \setminus \{x\}}(x) = \frac{1}{m-1} \sum_{x' \in X \setminus \{x\}} r^{-d} k\left(\frac{x' - x}{r}\right)$$

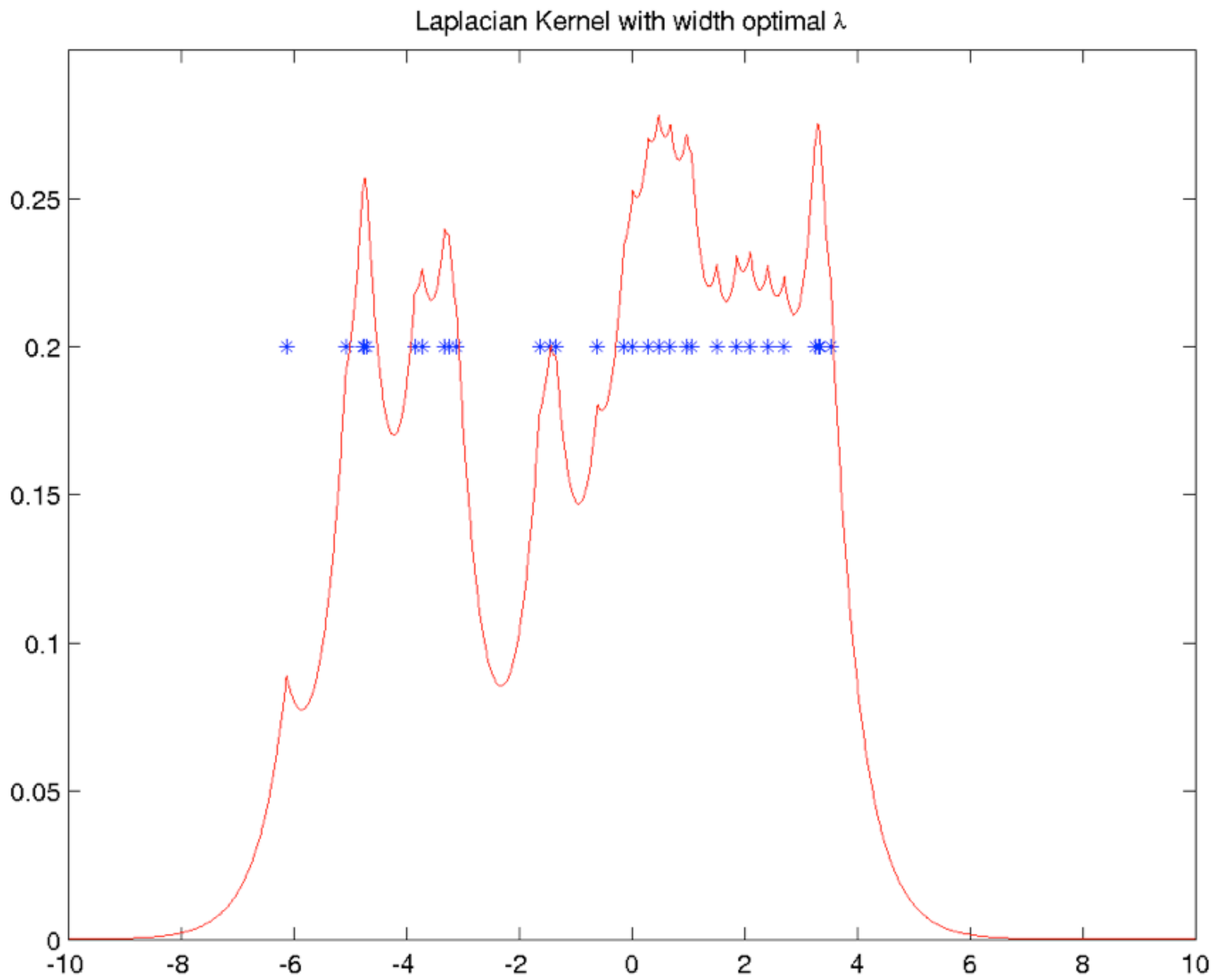
$$= \frac{m}{m-1}\left[\hat{p}(x) - m^{-1} r^{-d} k(0)\right]$$

$$\Longrightarrow \mathcal{L}[X] = m \log m/(m-1) + \sum_{x \in X} \log\left[\hat{p}(x) - m^{-1} r^{-d} k(0)\right]$$

Leave-one out estimate



Optimal estimate

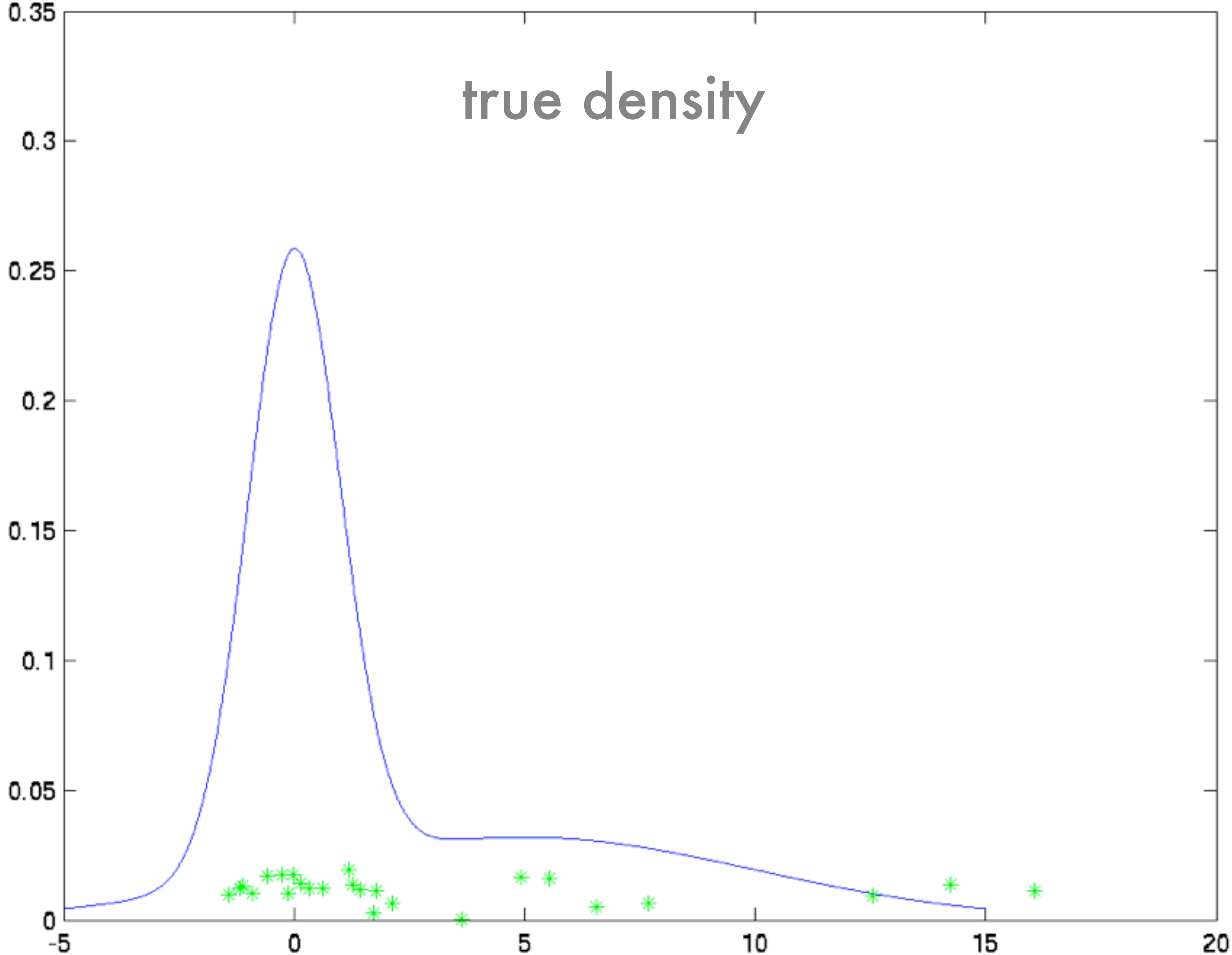


Silverman's rule

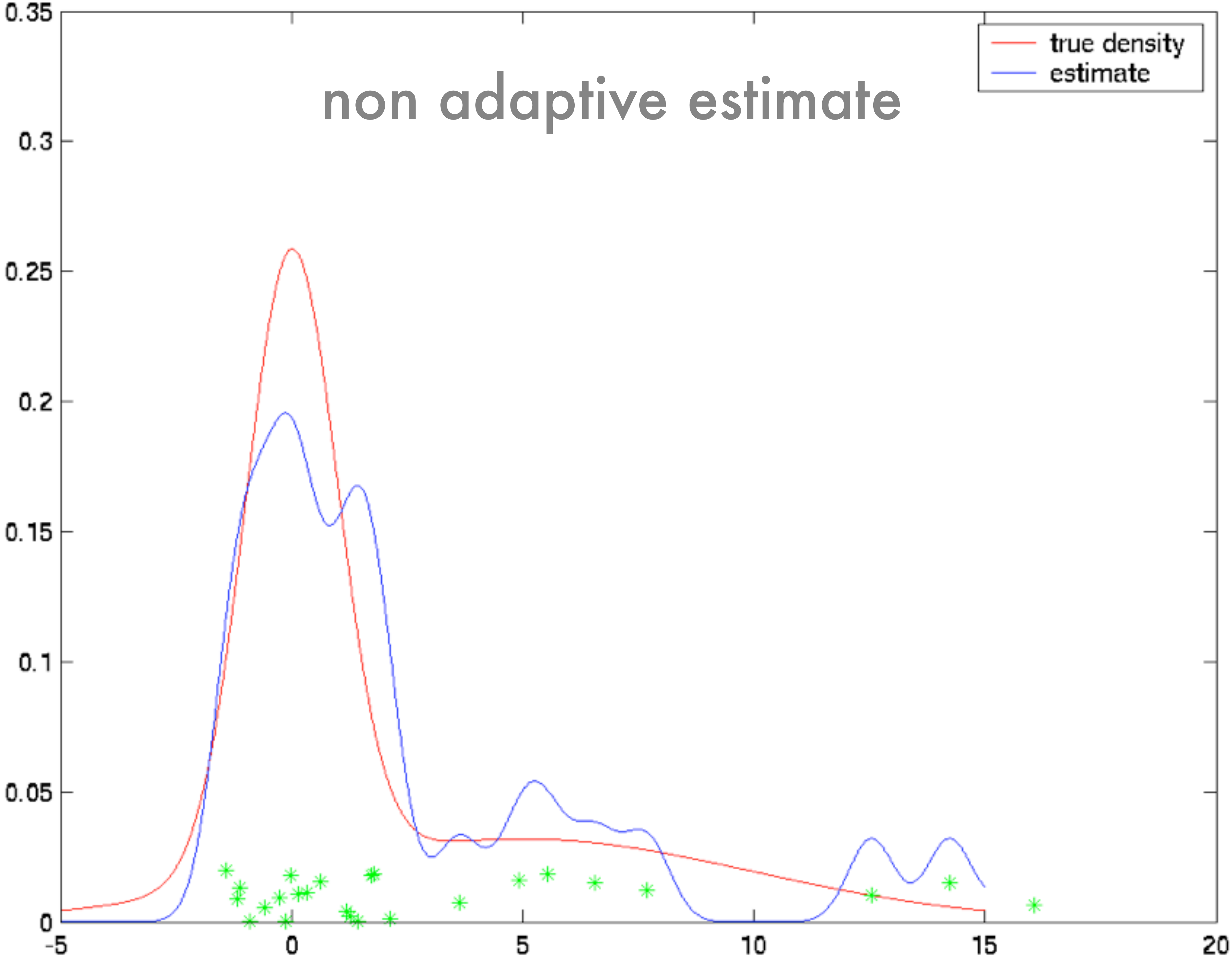
Silverman's rule

- Chicken and egg problem
  - Want wide kernel for low density region
  - Want narrow kernel where we have much data
  - Need density estimate to estimate density
- Simple hack
  Use average distance from k nearest neighbors

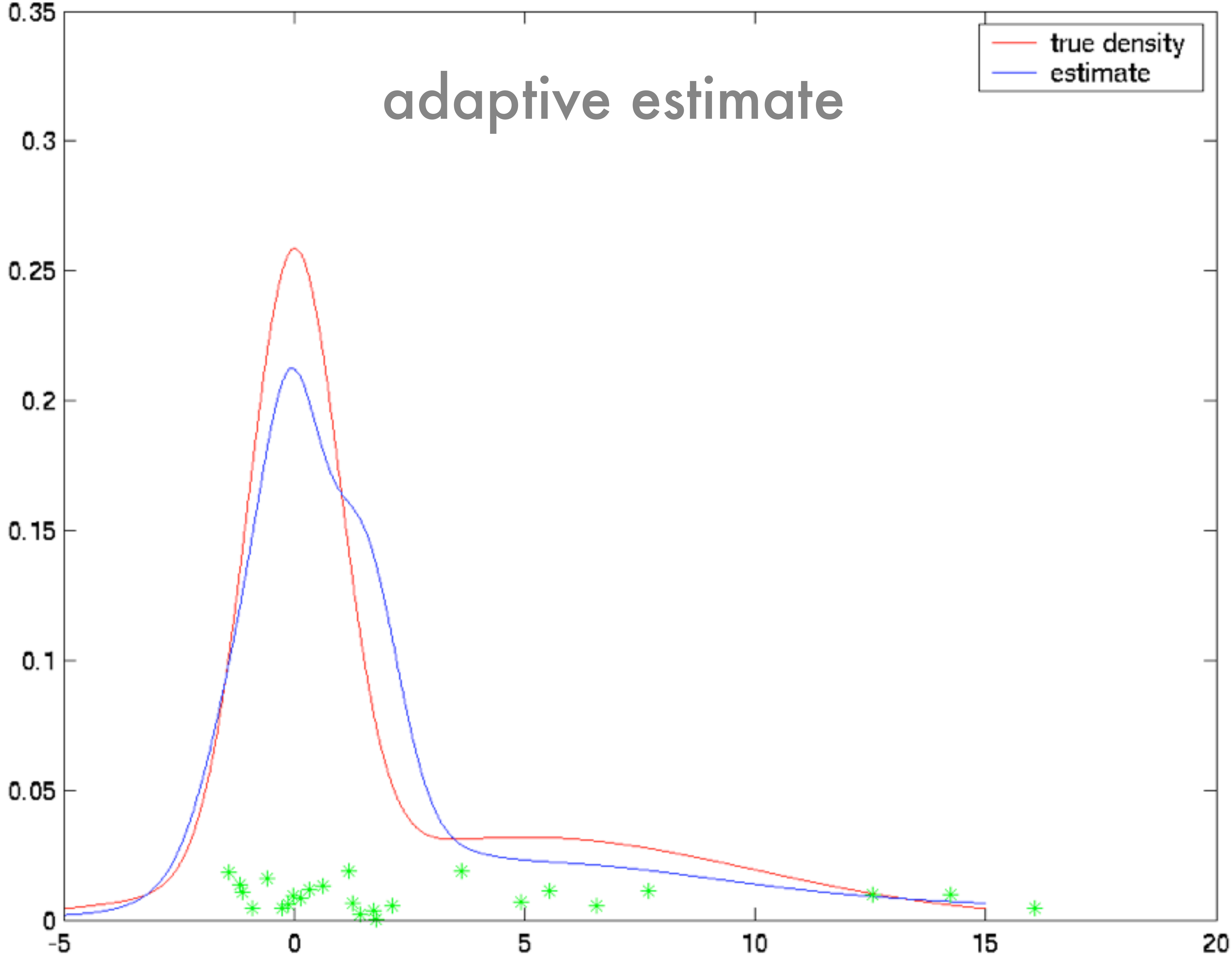
$$r_i = \frac{r}{k} \sum_{x \in \mathrm{NN}(x_i, k)} \|x_i - x\|$$

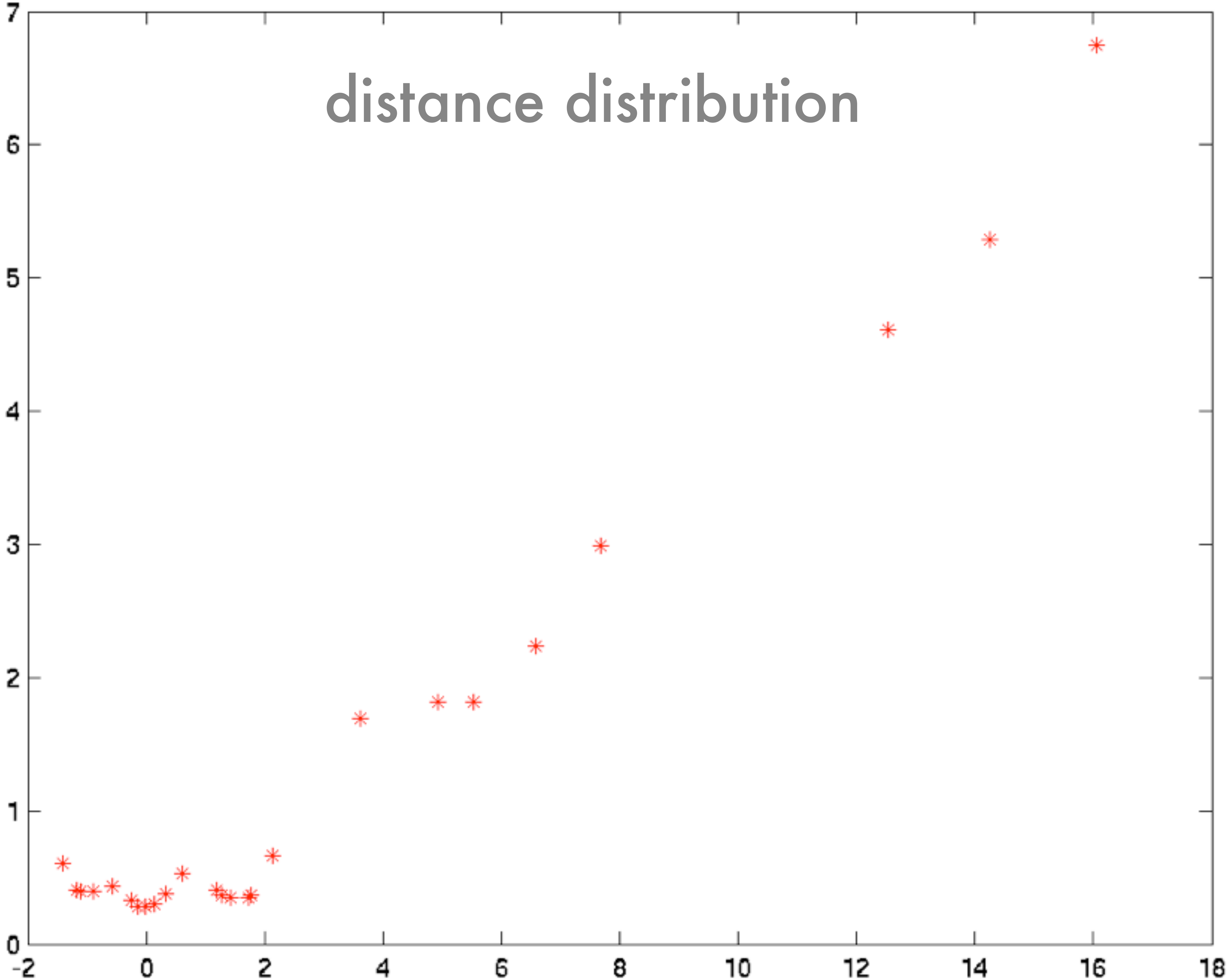


true density
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-5
0
5
10
15
20



non adaptive estimate
true density
estimate
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-5
0
5
10
15
20


adaptive estimate
true density
estimate
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-5
0
5
10
15
20


distance distribution
0
1
2
3
4
5
6
7
-2
0
2
4
6
8
10
12
14
16
18

Watson-Nadaraya estimator

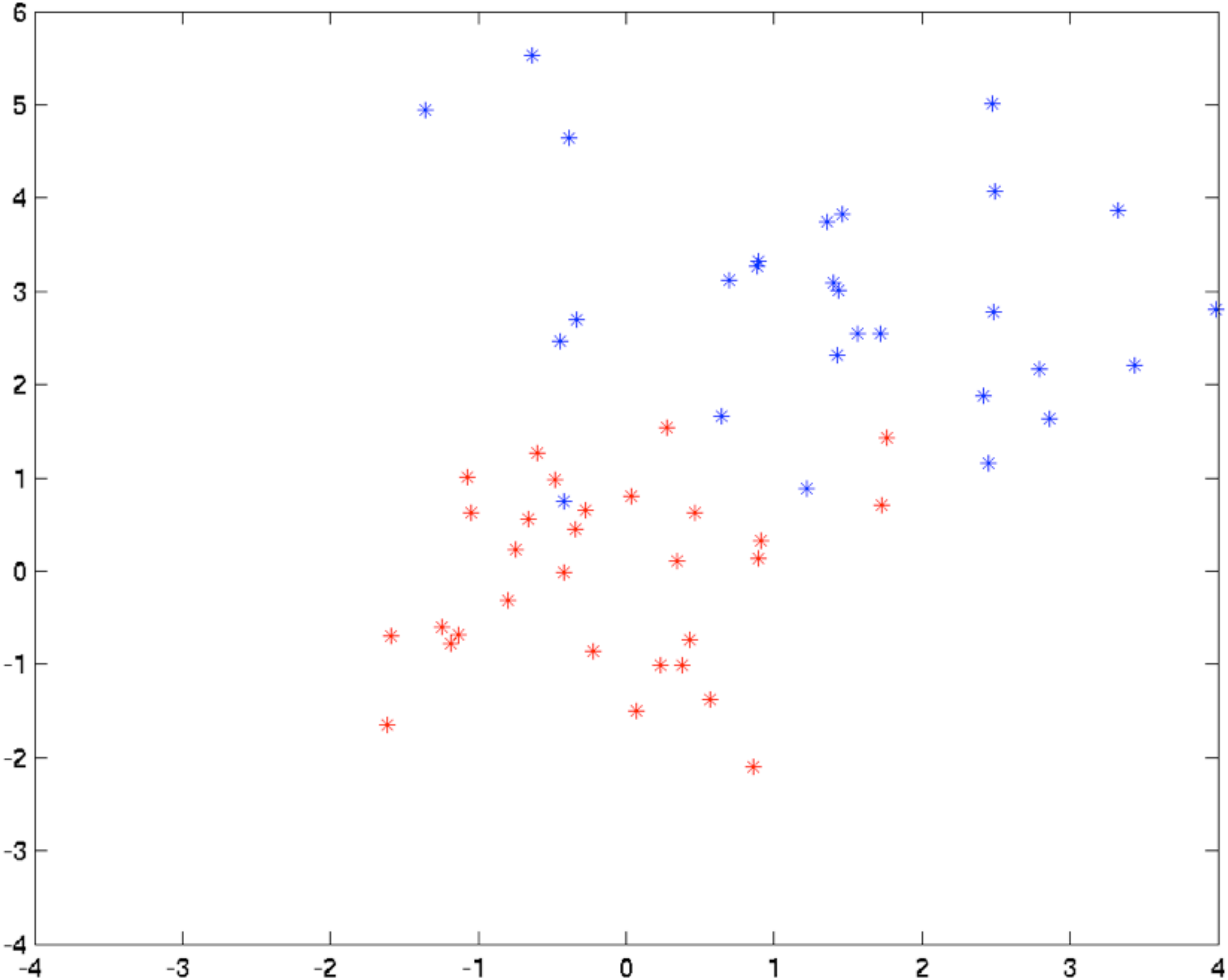
Weighted smoother

- Problem
  Given pairs (x_i, y_i) estimate $y|x$ for new x
- Idea
  Use distance weighted average of y_i

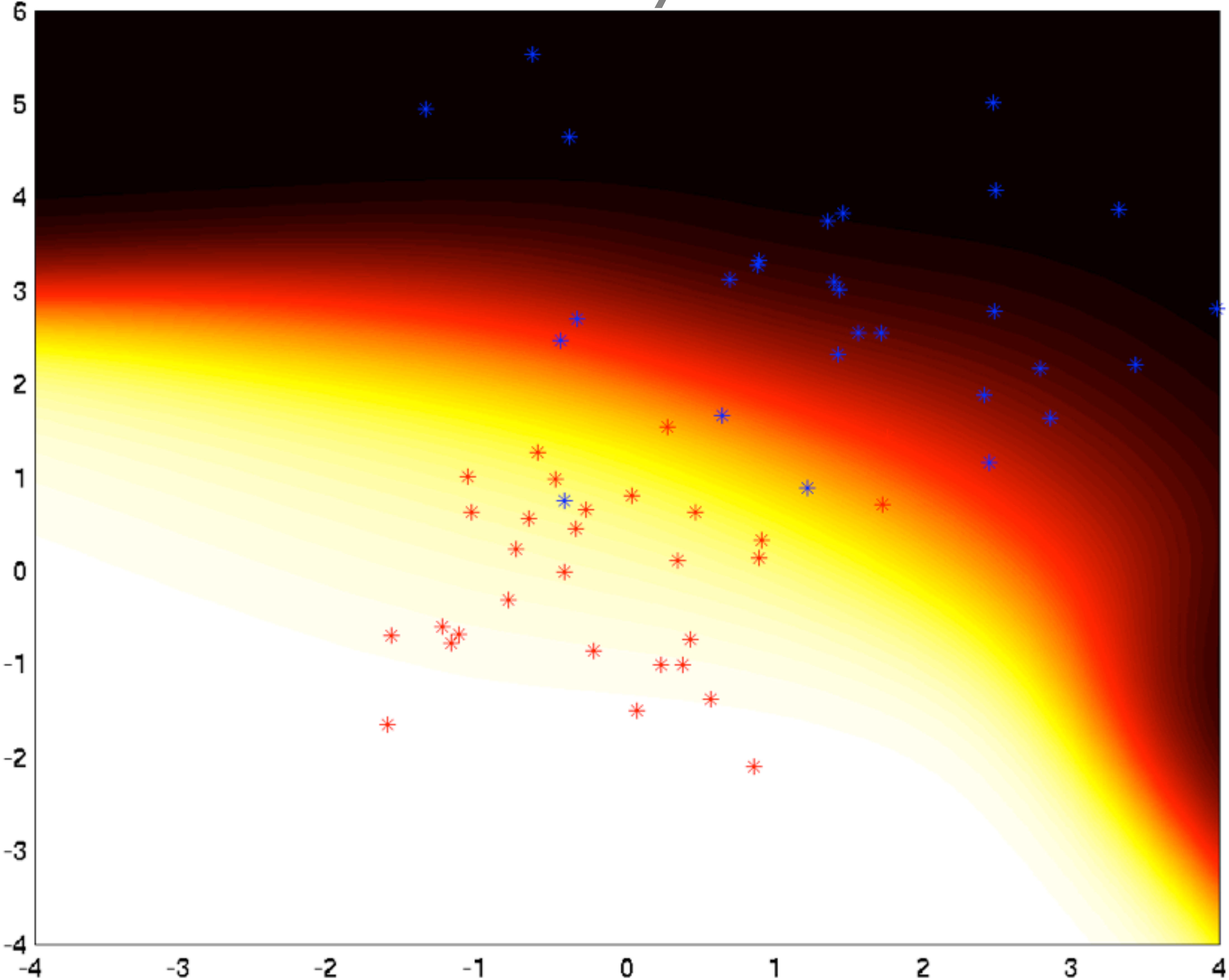
$$\hat{y}(x) = \sum_i y_i \frac{k_{x_i}(x)}{\sum_j k_{x_j}(x)} = \frac{\sum_i y_i k_{x_i}(x)}{\sum_j k_{x_j}(x)}$$

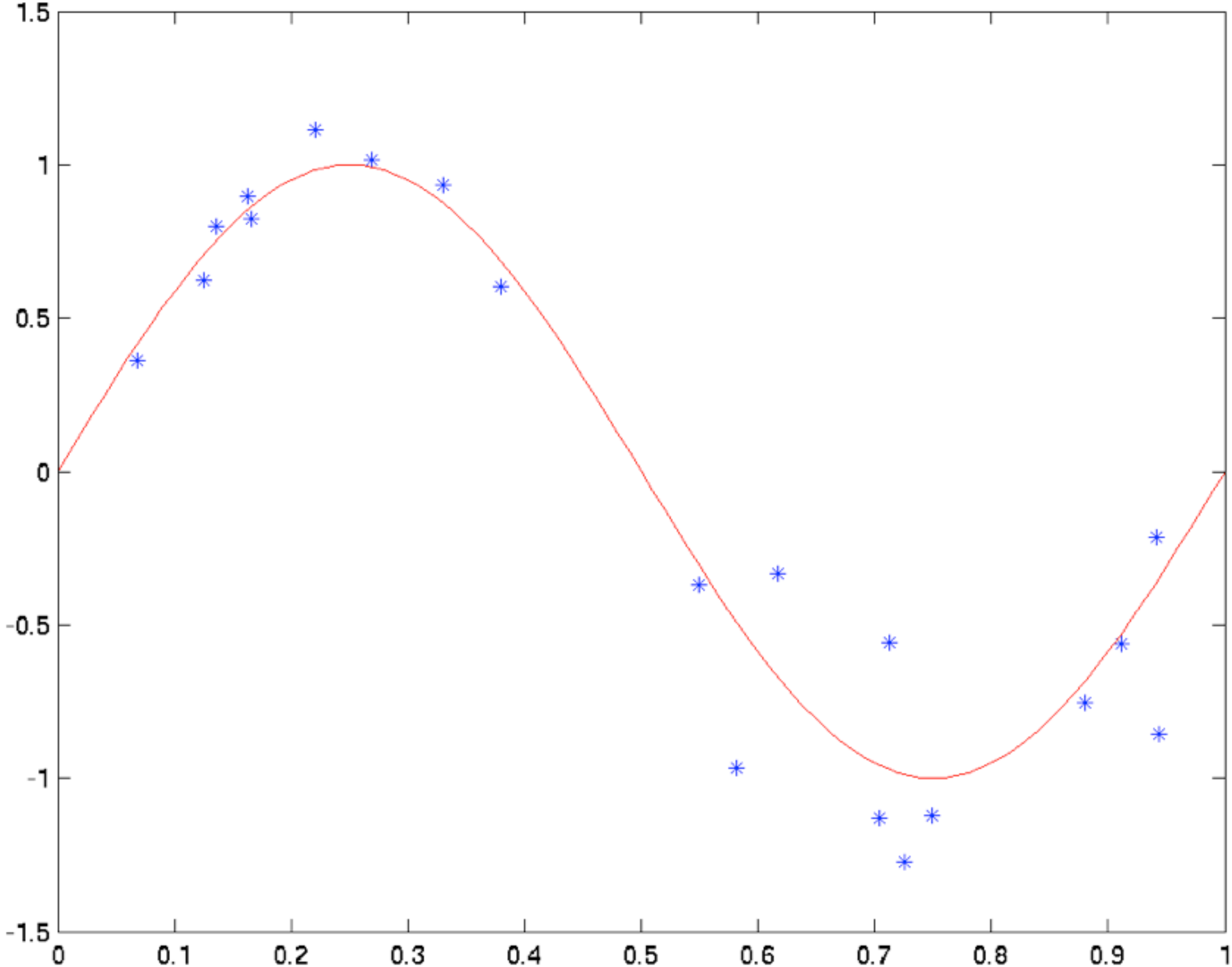
labels

local weights

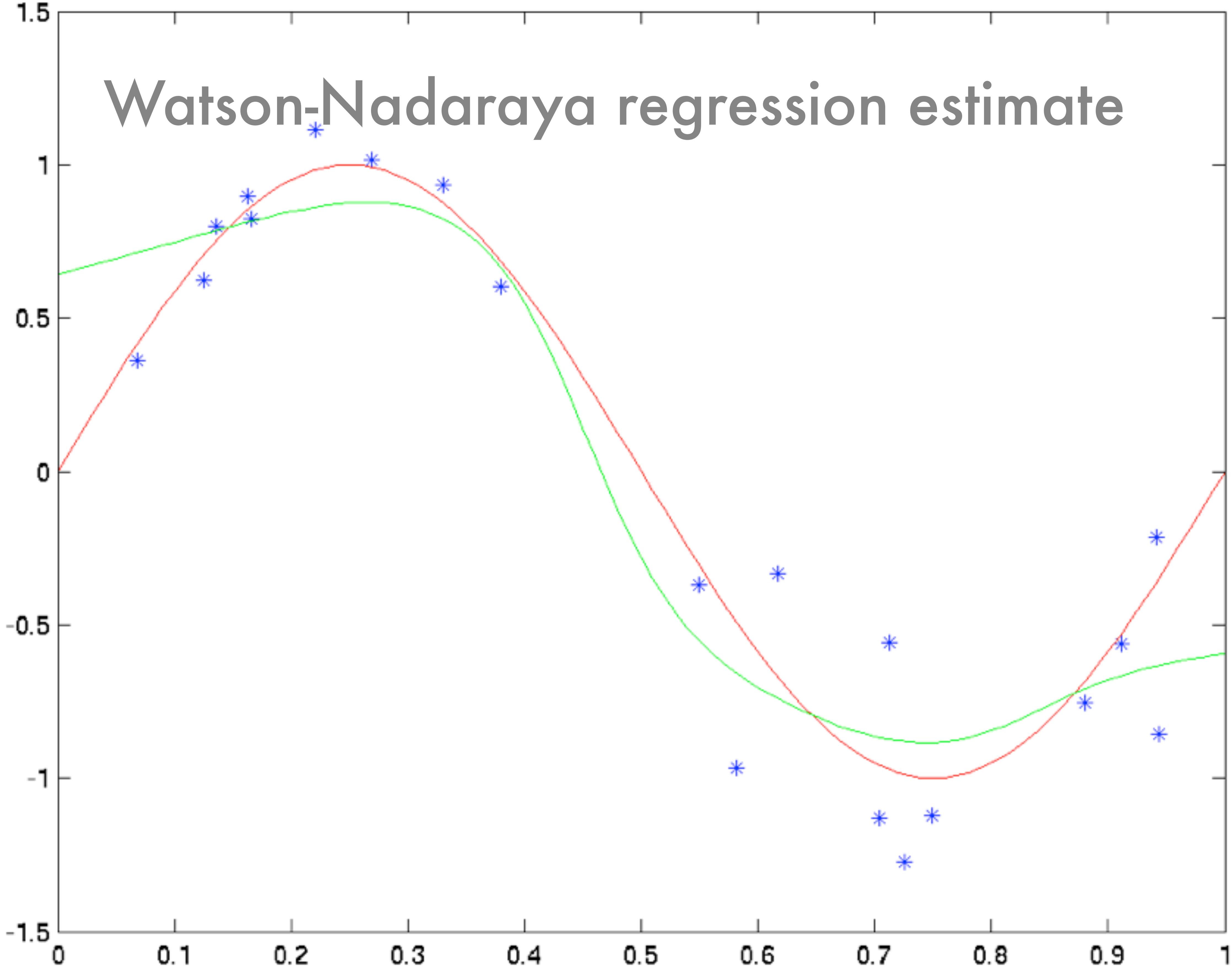

6
5
4
3
2
1
0
-1
-2
-3
-4
-4
-3
-2
-1
0
1
2
3
4

Watson-Nadaraya Classifier





1.5
1
0.5
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Watson-Nadaraya regression estimate
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

k-Nearest Neighbors

- Further simplification
  - Same weight for all nearest neighbors
  - Same number of neighbors everywhere
- Classification
  Use majority rule to estimate label
- Regression
  Use average for label

2.4 Exponential Families

Exponential Families

Exponential Families

- Density function

$$p(x;\theta) = \exp\left(\langle \phi(x), \theta \rangle - g(\theta)\right)$$

$$\text{where } g(\theta) = \log \sum_{x'} \exp\left(\langle \phi(x'), \theta \rangle\right)$$

Exponential Families

- Density function

$$p(x;\theta) = \exp\left(\langle \phi(x), \theta \rangle - g(\theta)\right)$$

$$\text{where } g(\theta) = \log \sum_{x'} \exp\left(\langle \phi(x'), \theta \rangle\right)$$

- Log partition function generates cumulants

$$\partial_\theta g(\theta) = \mathbf{E}\left[\phi(x)\right]$$

$$\partial^2_\theta g(\theta) = \mathrm{Var}\left[\phi(x)\right]$$

Exponential Families

- Density function

$$p(x;\theta) = \exp\left(\langle \phi(x), \theta \rangle - g(\theta)\right)$$
$$\text{where } g(\theta) = \log \sum_{x'} \exp\left(\langle \phi(x'), \theta \rangle\right)$$

- Log partition function generates cumulants

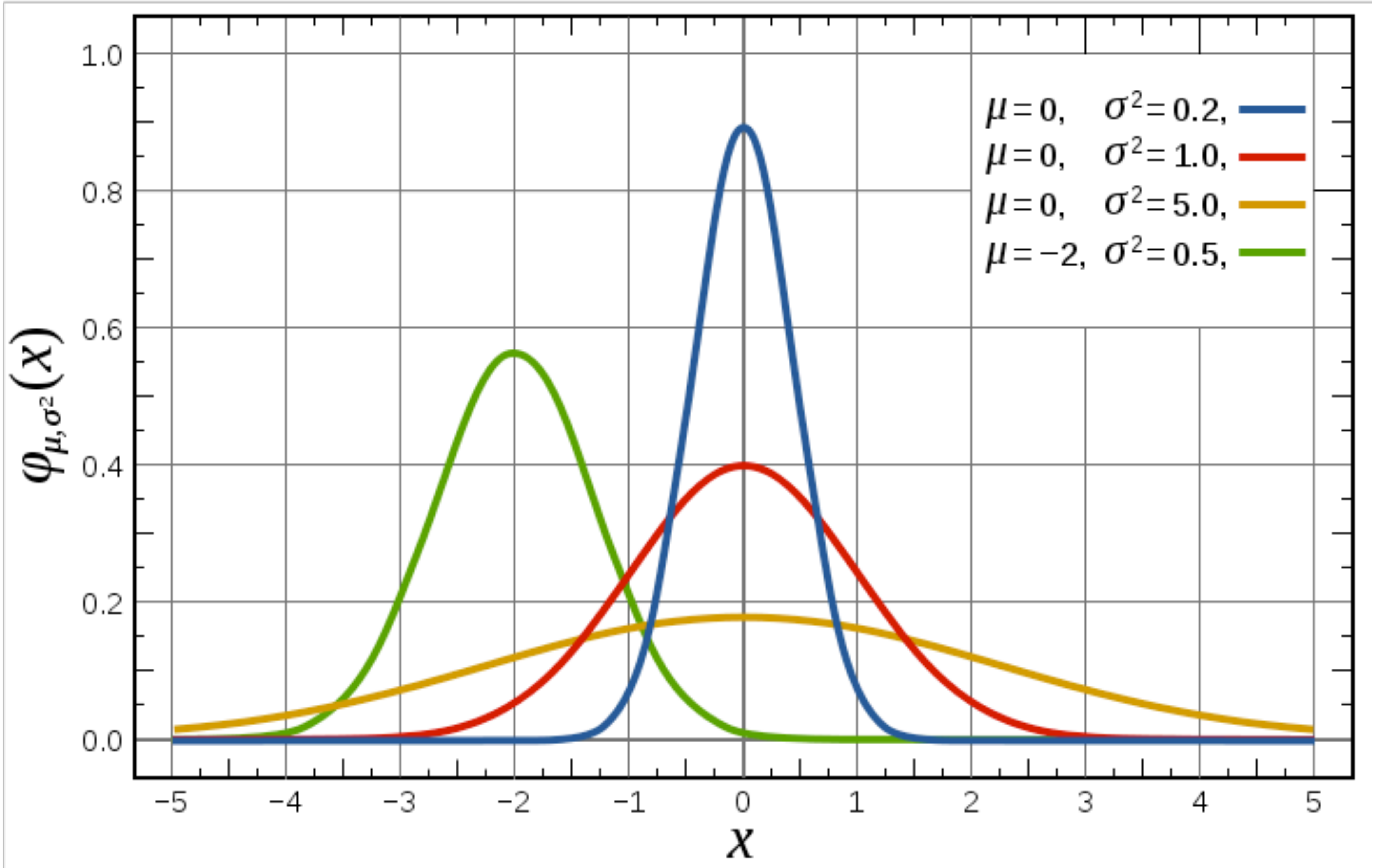
$$\partial_\theta g(\theta) = \mathbf{E}\left[\phi(x)\right]$$
$$\partial_\theta^2 g(\theta) = \mathrm{Var}\left[\phi(x)\right]$$

- g is convex (second derivative is p.s.d.)

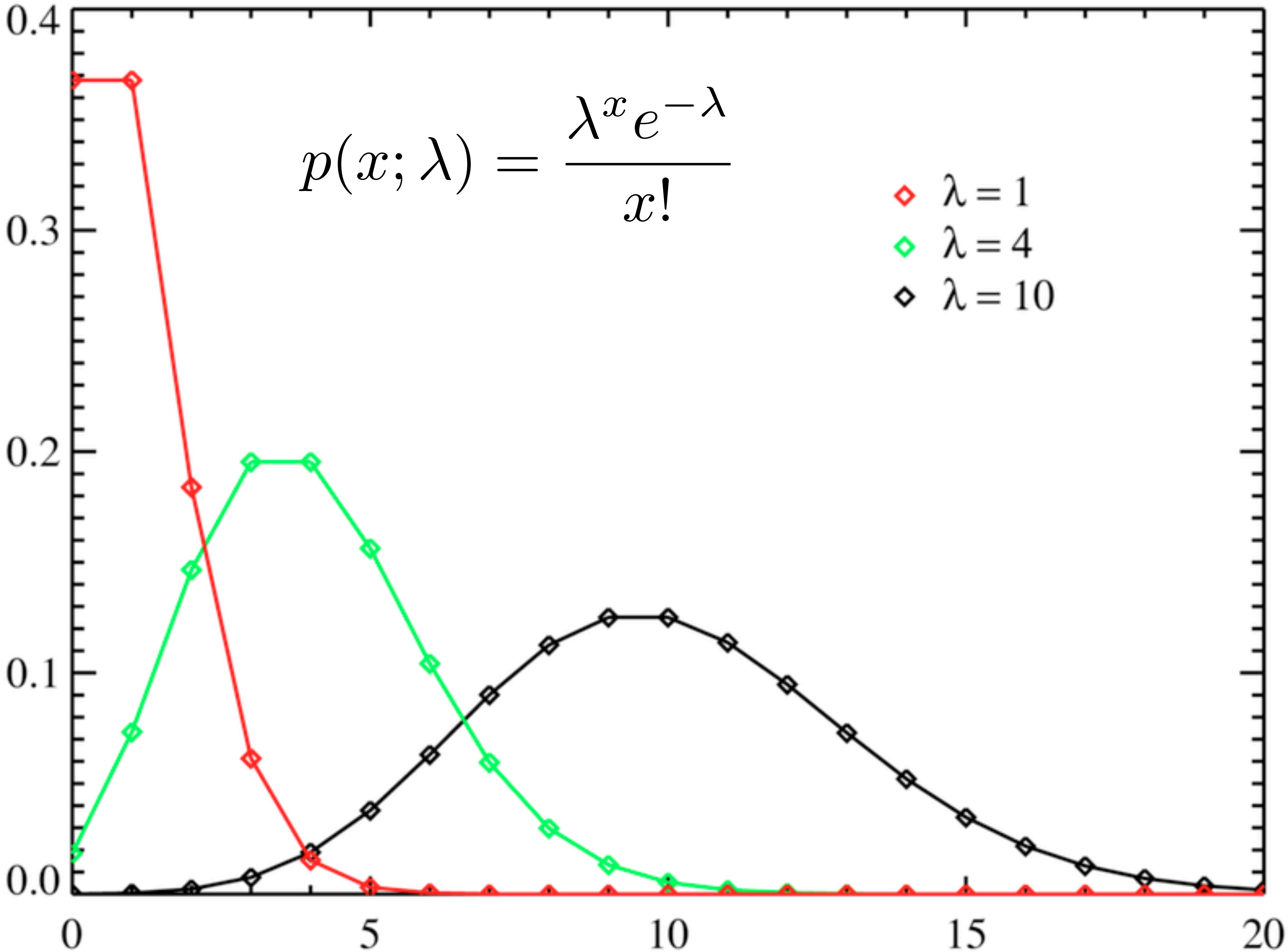
Examples

- Binomial Distribution $\phi(x) = x$
- Discrete Distribution $\phi(x) = e_x$
  (e_x is unit vector for x)
- Gaussian $\phi(x) = \left(x, \frac{1}{2} x x^\top\right)$
- Poisson (counting measure 1/x!) $\phi(x) = x$
- Dirichlet, Beta, Gamma, Wishart, ...

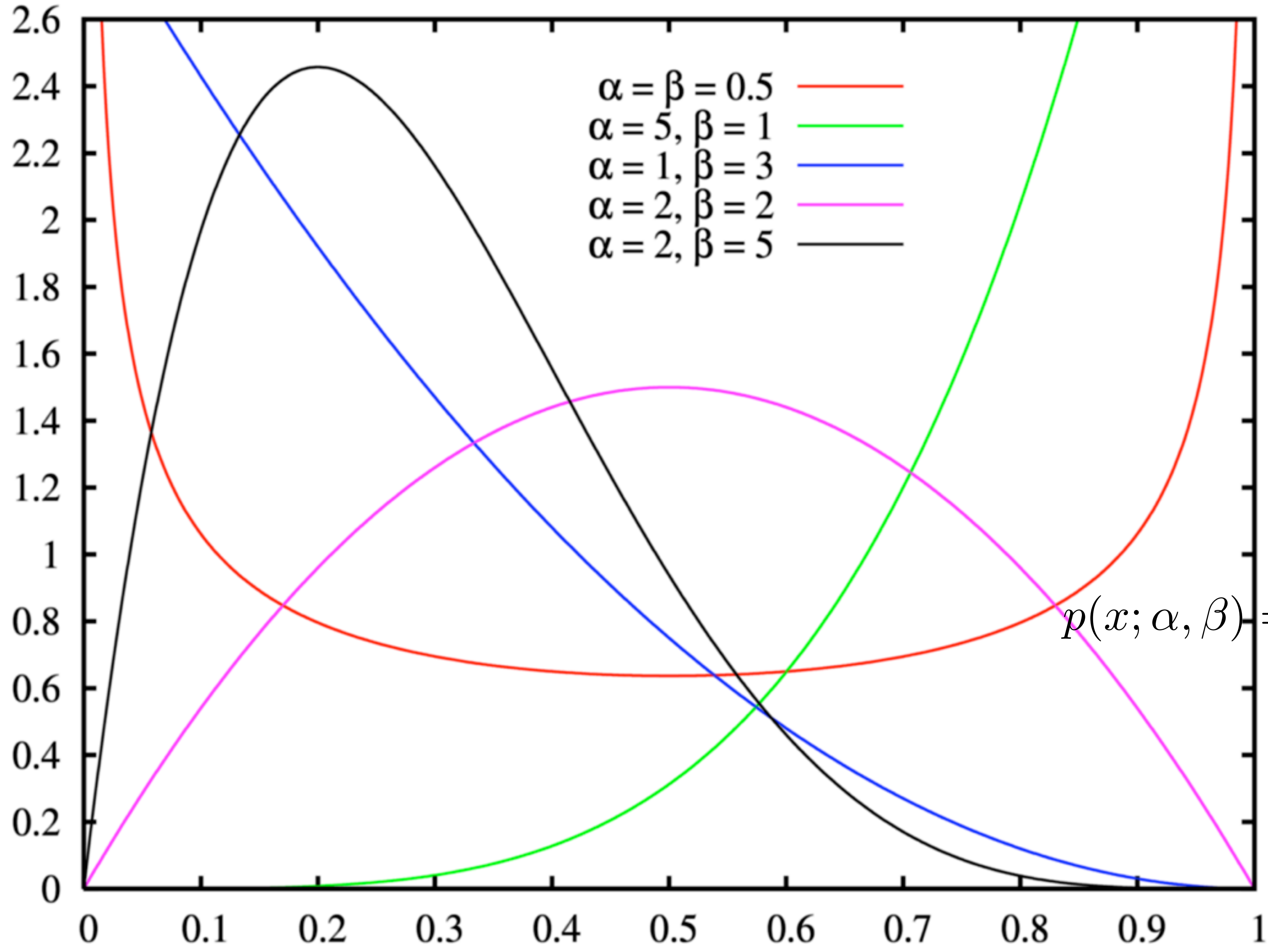
Normal Distribution



Poisson Distribution

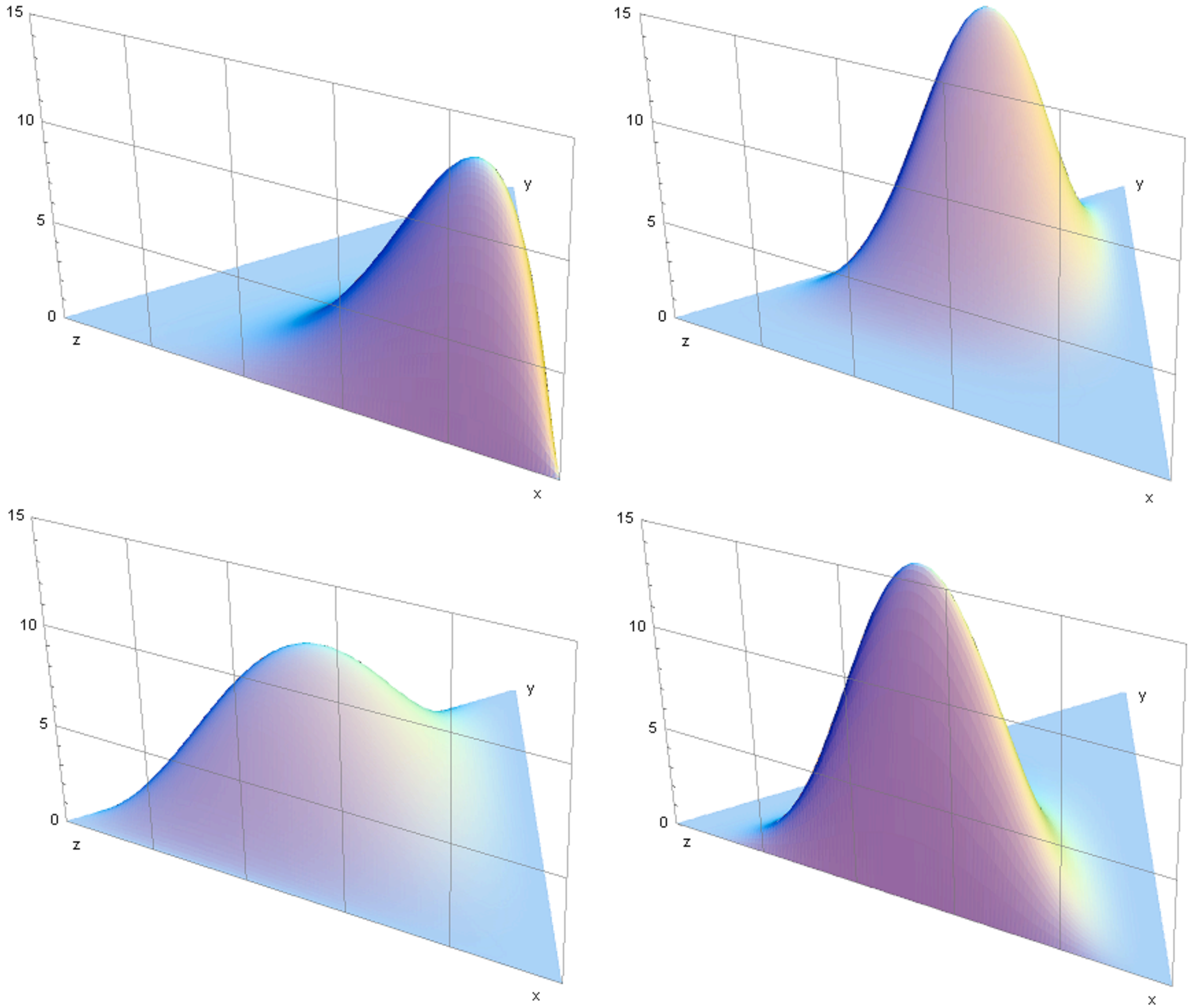


Beta Distribution



$$p(x;\alpha,\beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}$$

Dirichlet Distribution



... this is a distribution over distributions ...

Maximum Likelihood

Maximum Likelihood

- Negative log-likelihood

$$-\log p(X;\theta) = \sum_{i=1}^{n} g(\theta) - \langle \phi(x_i), \theta \rangle$$

Maximum Likelihood

- Negative log-likelihood

$$-\log p(X;\theta) = \sum_{i=1}^{n} g(\theta) - \langle \phi(x_i), \theta \rangle$$

- Taking derivatives

mean

empirical average

$$-\partial_\theta \log p(X;\theta) = m \left[\mathbf{E}[\phi(x)] - \frac{1}{m} \sum_{i=1}^{n} \phi(x_i) \right]$$

We pick the parameter such that the distribution matches the empirical average.

Conjugate Priors

- Unless we have lots of data estimates are weak
- Usually we have an idea of what to expect

$$p(\theta|X) \propto p(X|\theta) \cdot p(\theta)$$

we might even have 'seen' such data before

- Solution: add 'fake' observations

$$p(\theta) \propto p(X_{\text{fake}}|\theta) \text{ hence } p(\theta|X) \propto p(X|\theta)p(X_{\text{fake}}|\theta) = p(X \cup X_{\text{fake}}|\theta)$$

- Inference (generalized Laplace smoothing)

$$\frac{1}{n}\sum_{i=1}^{n}\phi(x_i) \longrightarrow \frac{1}{n+m}\sum_{i=1}^{n}\phi(x_i) + \frac{m}{n+m}\mu_0$$

fake count (m)

fake mean (μ_0)

Example: Gaussian Estimation

- Sufficient statistics: x, x^2
- Mean and variance given by

$$\mu = \mathbf{E}_x[x] \text{ and } \sigma^2 = \mathbf{E}_x[x^2] - \mathbf{E}^2_x[x]$$

- Maximum Likelihood Estimate

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \text{ and } \sigma^2 = \frac{1}{n}\sum_{i=1}^{n} x_i^2 - \hat{\mu}^2$$

- Maximum a Posteriori Estimate

smoother

$$\hat{\mu} = \frac{1}{n+n_0}\sum_{i=1}^{n} x_i \text{ and } \sigma^2 = \frac{1}{n+n_0}\sum_{i=1}^{n} x_i^2 + \frac{n_0}{n+n_0}\mathbf{1} - \hat{\mu}^2$$

smoother

Collapsing

- Conjugate priors

$$p(\theta) \propto p(X_{\text{fake}}|\theta)$$

Hence we know how to compute normalization

- Prediction

$$p(x|X) = \int p(x|\theta)p(\theta|X)d\theta$$

$$\propto \int p(x|\theta)p(X|\theta)p(X_{\text{fake}}|\theta)d\theta$$

$$= \int p(\{x\} \cup X \cup X_{\text{fake}}|\theta)d\theta$$

(Beta, binomial)
(Dirichlet, multinomial)
(Gamma, Poisson)
(Wishart, Gauss)

look up closed form expansions

http://en.wikipedia.org/wiki/Exponential_family

Conjugate Prior in action

$$m_i = m \cdot [\mu_0]_i$$

$$p(x = i) = \frac{n_i}{n} \longrightarrow p(x = i) = \frac{n_i + m_i}{n + m}$$

Outcome	1	2	3	4	5	6
Counts	3	6	2	1	4	4
MLE	0.15	0.30	0.10	0.05	0.20	0.20
MAP ($m_0 = 6$)	0.15	0.27	0.12	0.08	0.19	0.19
MAP ($m_0 = 100$)	0.16	0.19	0.16	0.15	0.17	0.17

Conjugate Prior in action

$m_i = m \cdot [\mu_0]_i$

- **Discrete Distribution**

$$p(x = i) = \frac{n_i}{n} \longrightarrow p(x = i) = \frac{n_i + m_i}{n + m}$$

- **Tossing a dice**

Outcome	1	2	3	4	5	6
Counts	3	6	2	1	4	4
MLE	0.15	0.30	0.10	0.05	0.20	0.20
MAP ($m_0 = 6$)	0.15	0.27	0.12	0.08	0.19	0.19
MAP ($m_0 = 100$)	0.16	0.19	0.16	0.15	0.17	0.17

Conjugate Prior in action

$$m_i = m \cdot [\mu_0]_i$$

- Discrete Distribution

$$p(x = i) = \frac{n_i}{n} \longrightarrow p(x = i) = \frac{n_i + m_i}{n + m}$$

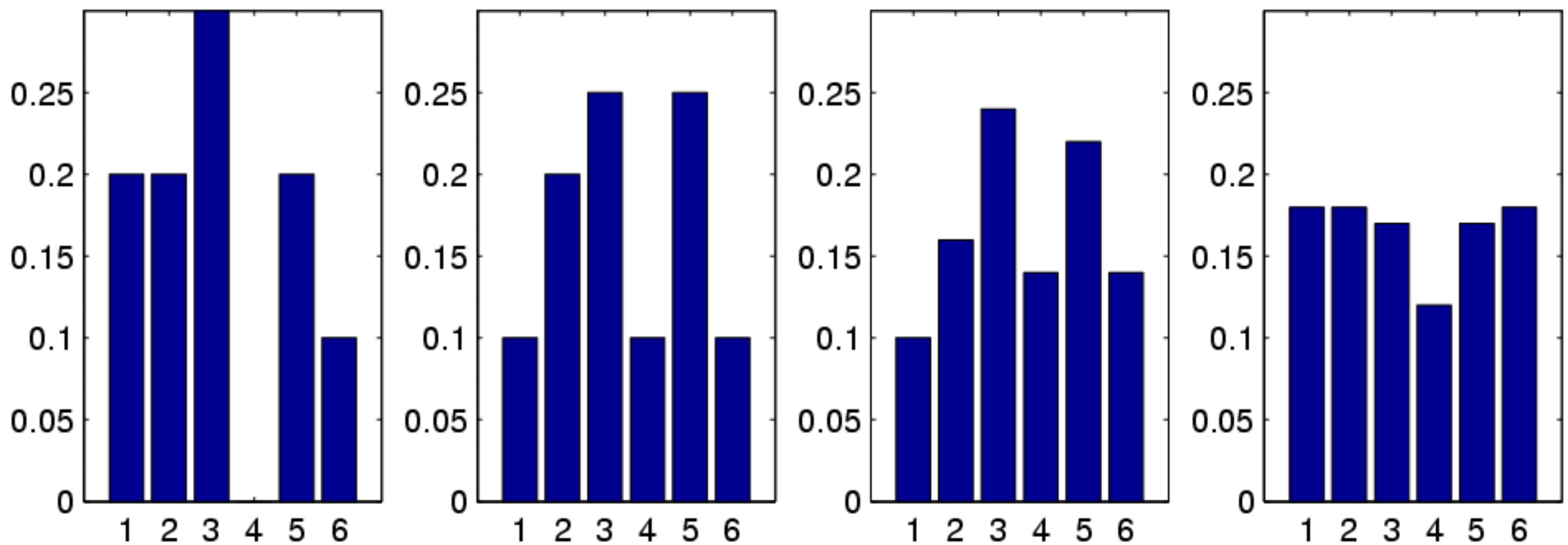
- Tossing a dice

Outcome	1	2	3	4	5	6
Counts	3	6	2	1	4	4
MLE	0.15	0.30	0.10	0.05	0.20	0.20
MAP ($m_0 = 6$)	0.15	0.27	0.12	0.08	0.19	0.19
MAP ($m_0 = 100$)	0.16	0.19	0.16	0.15	0.17	0.17

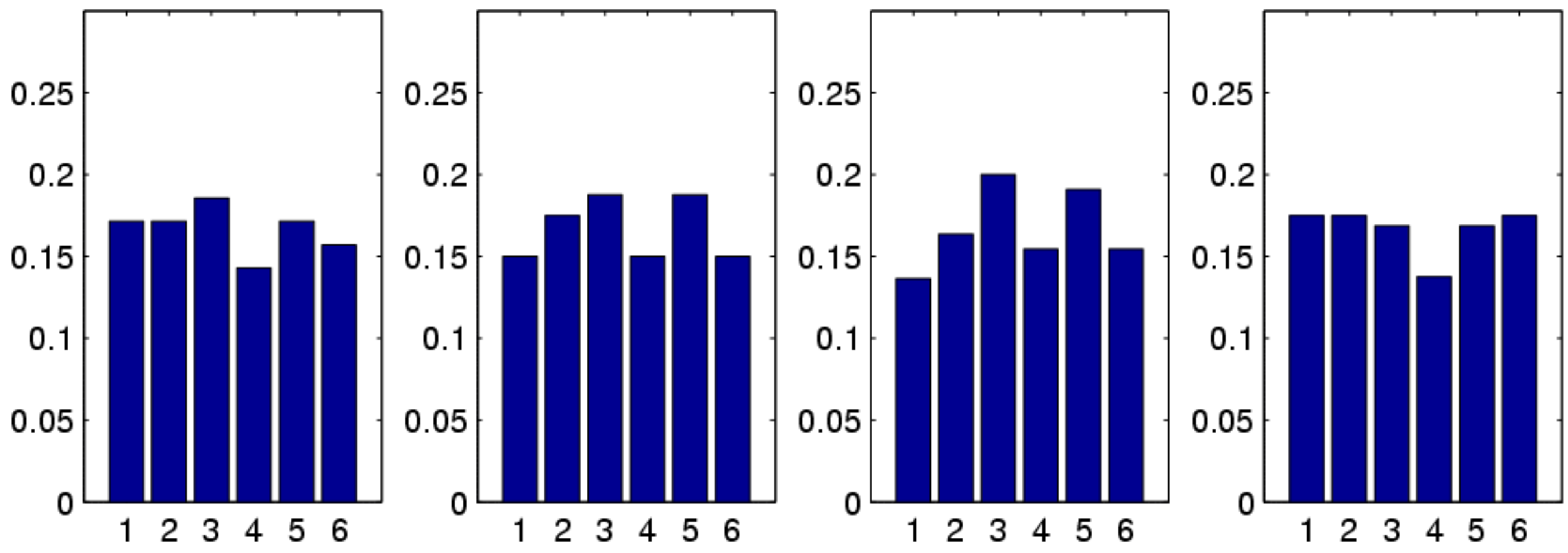
- Rule of thumb
  need 10 data points (or prior) per parameter

Honest dice

MLE



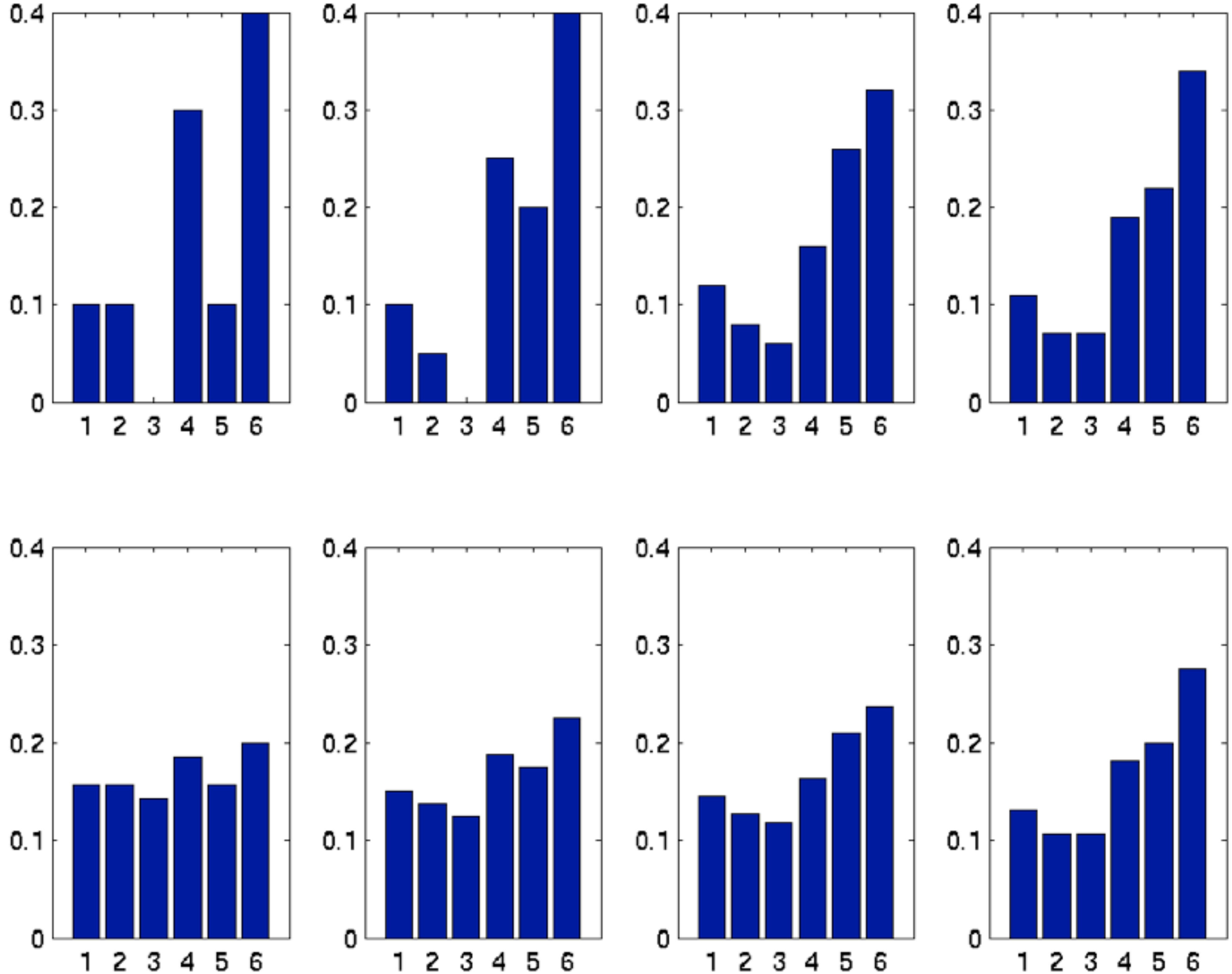
MAP



Tainted dice

MLE

MAP



Priors (part deux)

- **Parameter smoothing**

$$p(\theta) \propto \exp(-\lambda \|\theta\|_1) \text{ or } p(\theta) \propto \exp(-\lambda \|\theta\|_2^2)$$

- **Posterior**

$$p(\theta|x) \propto \prod_{i=1}^{m} p(x_i|\theta)p(\theta)$$

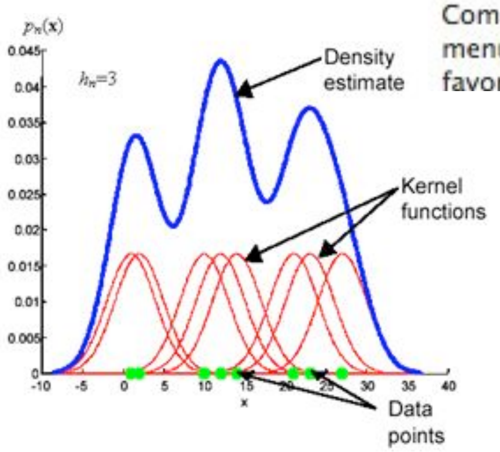
$$\propto \exp\left(\sum_{i=1}^{m} \langle \phi(x_i), \theta \rangle - mg(\theta) - \frac{1}{2\sigma^2} \|\theta\|_2^2\right)$$

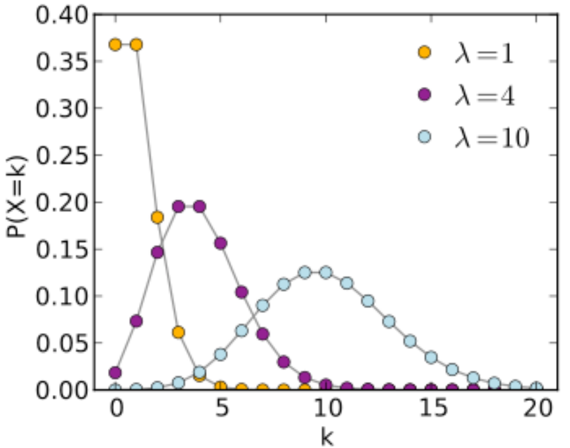
- **Convex optimization problem (MAP estimation)**

$$\underset{\theta}{\text{minimize}}\, g(\theta) - \left\langle \frac{1}{m} \sum_{i=1}^{m} \phi(x_i), \theta \right\rangle + \frac{1}{2m\sigma^2} \|\theta\|_2^2$$

Statistics

- Probabilities
  - Bayes rule, Dependence, independence, conditional probabilities
  - Priors, Naive Bayes classifier
- Tail bounds
  - Chernoff, Hoeffding, Chebyshev, Gaussian
  - A/B testing
- Kernel density estimation
  - Parzen windows, Nearest neighbors, Watson-Nadaraya estimator
- Exponential families
  - Gaussian, multinomial, Poisson
  - Conjugate distributions and smoothing, integrating out





Further reading

- Manuscript (book chapters 1 and 2)
  http://alex.smola.org/teaching/berkeley2012/slides/chapter1_2.pdf