DATA221 Intro Machine Learning
02 objective function

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THE UNIVERSITY OF CHICAGO

TECHNOLOGY

That smiling LinkedIn profile face might be a computer-generated fake

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SHANNON BOND

Caught in the wild!

And for the noble, purpose allowing salespeople to send spam with fewer constraints!

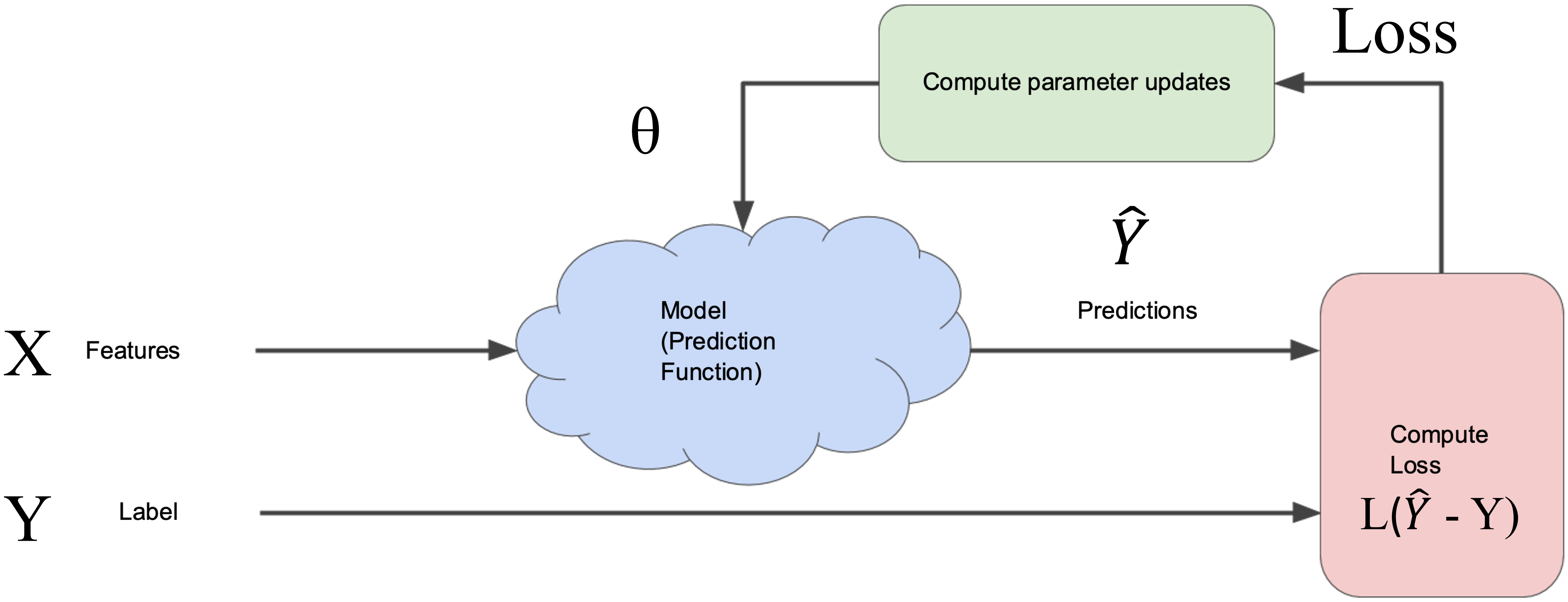
Some of the likely AI-generated faces from fake LinkedIn profiles identified by Stanford University researchers. The central positioning of the eyes is a telltale sign of a computer-created face. Click on the animation to pause.

Source: Stanford Internet Observatory

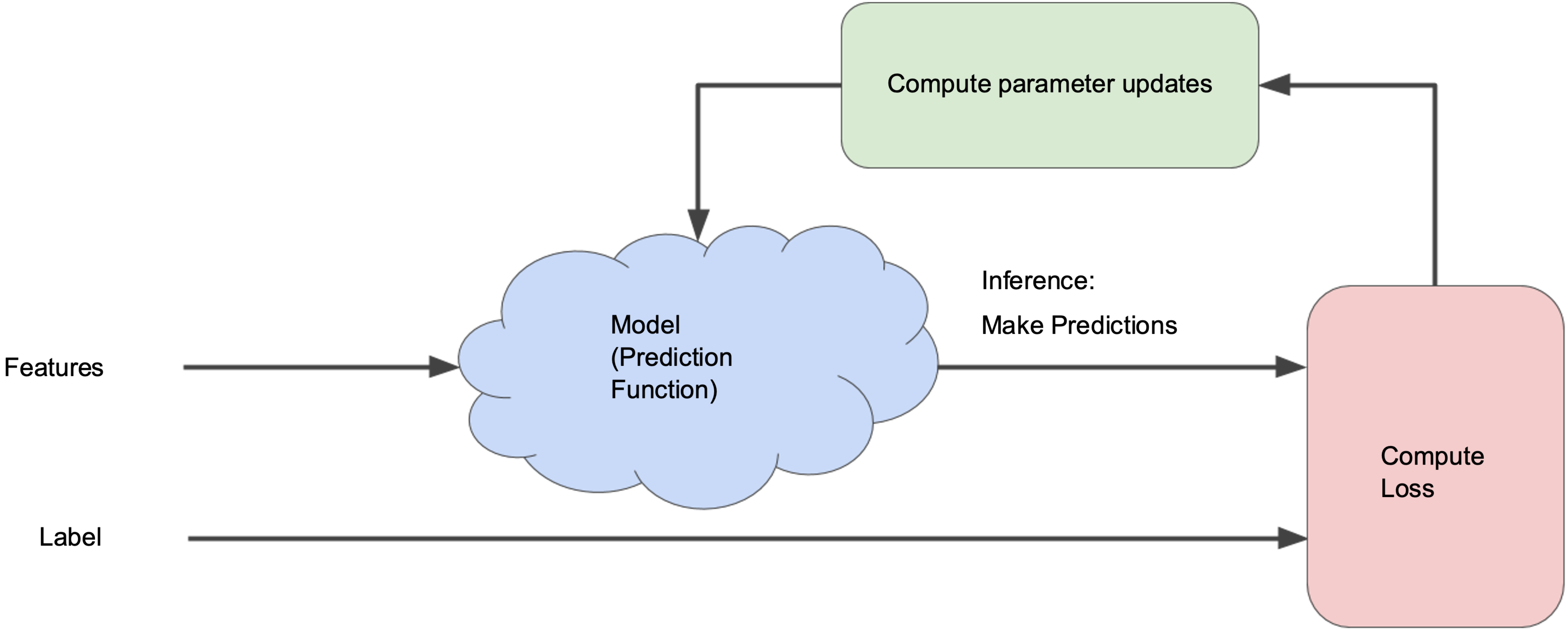
Credit: Connie Hanzhang Jin/NPR

https://www.npr.org/2022/03/27/1088140809/fake-linkedin-profiles

Fairy dust picture of optimization

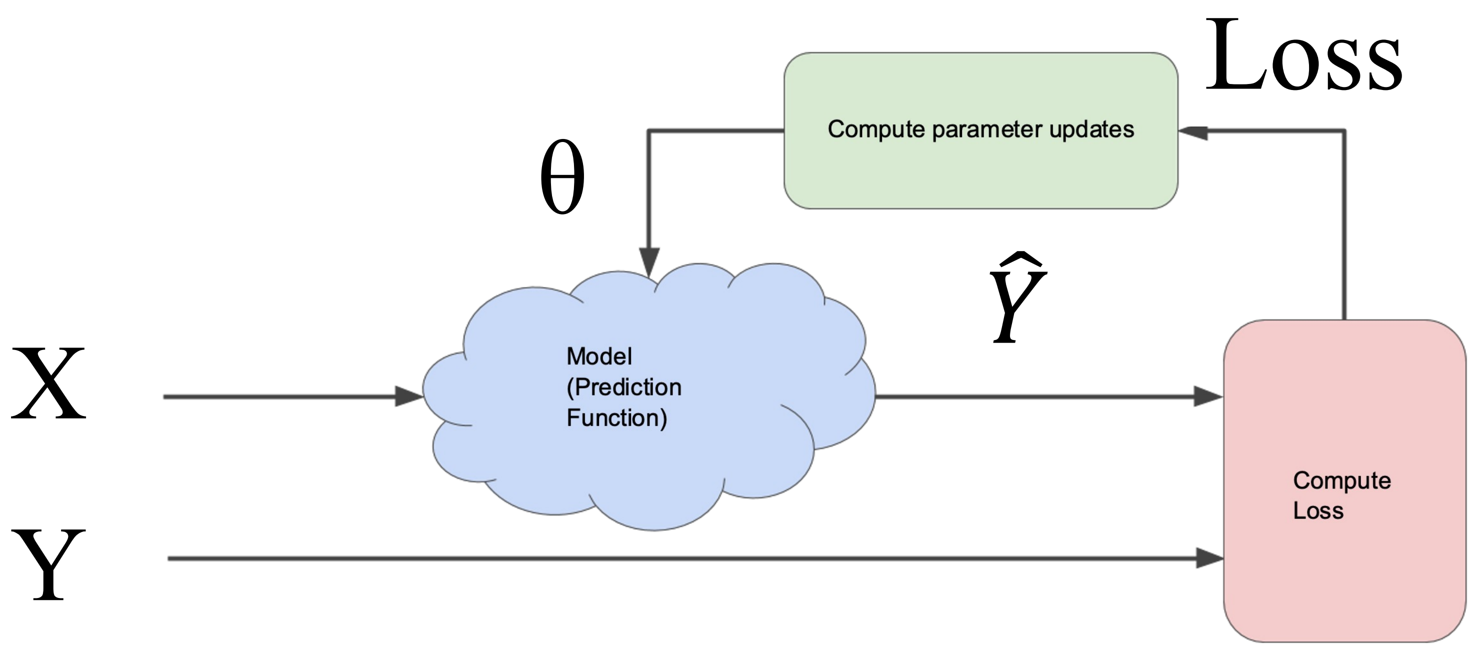


Fairy dust picture of optimization



Argmin symmetries

$$\hat{\theta} = \text{argmin}_{\theta}\ L(\theta,\ X,\ Y)$$



This metafunction has some symmetries:

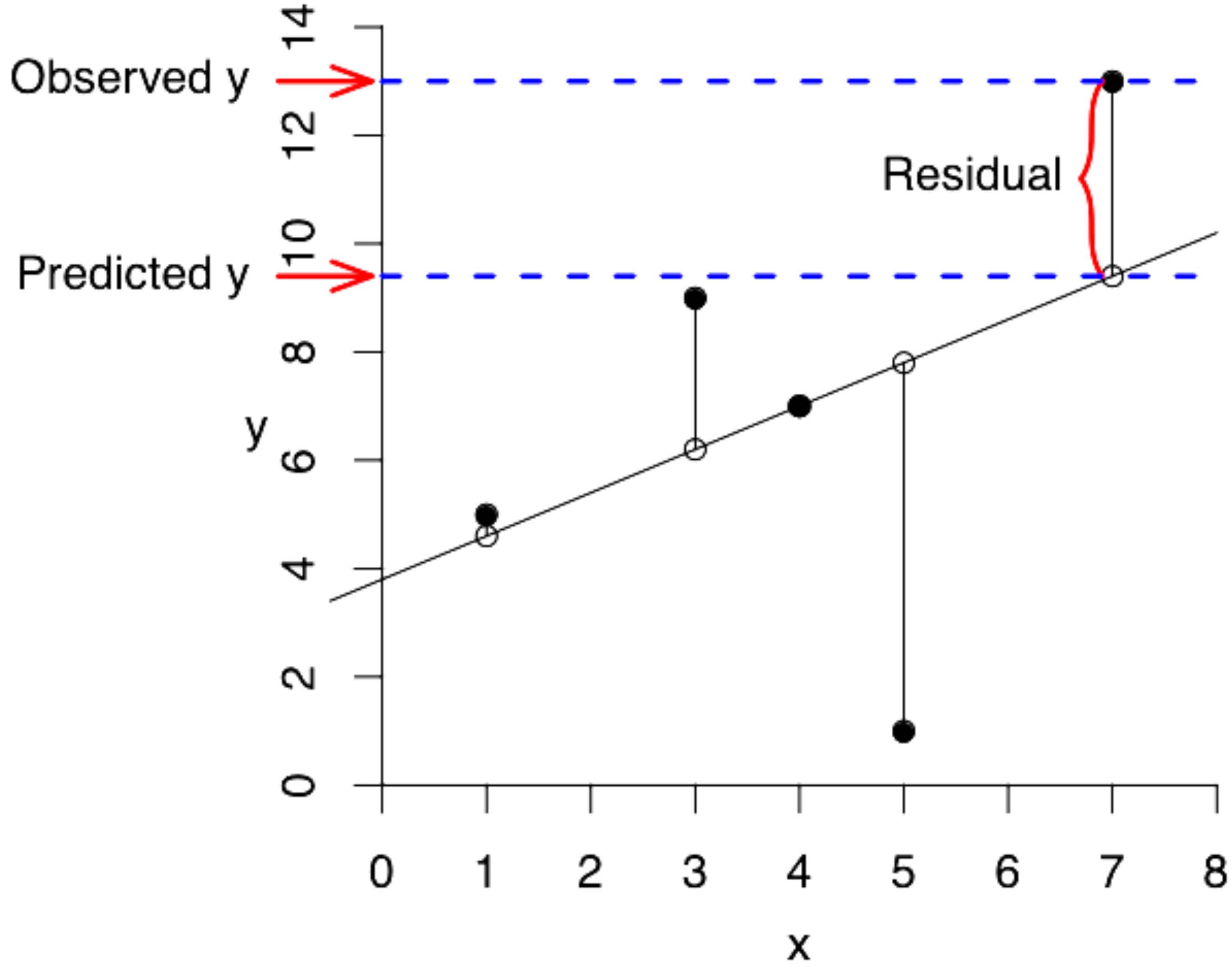
L+c has same argmin as L

cL has same argmin as L

L^2, abs(L), $L^{1/2}$ same argmin

log(L) has the same argmin if L isn't outside its domain

“Regression” = prediction of values



Summed squared error

$$SSE = \Sigma\ (\hat{y}_i - y_i\ )^2$$

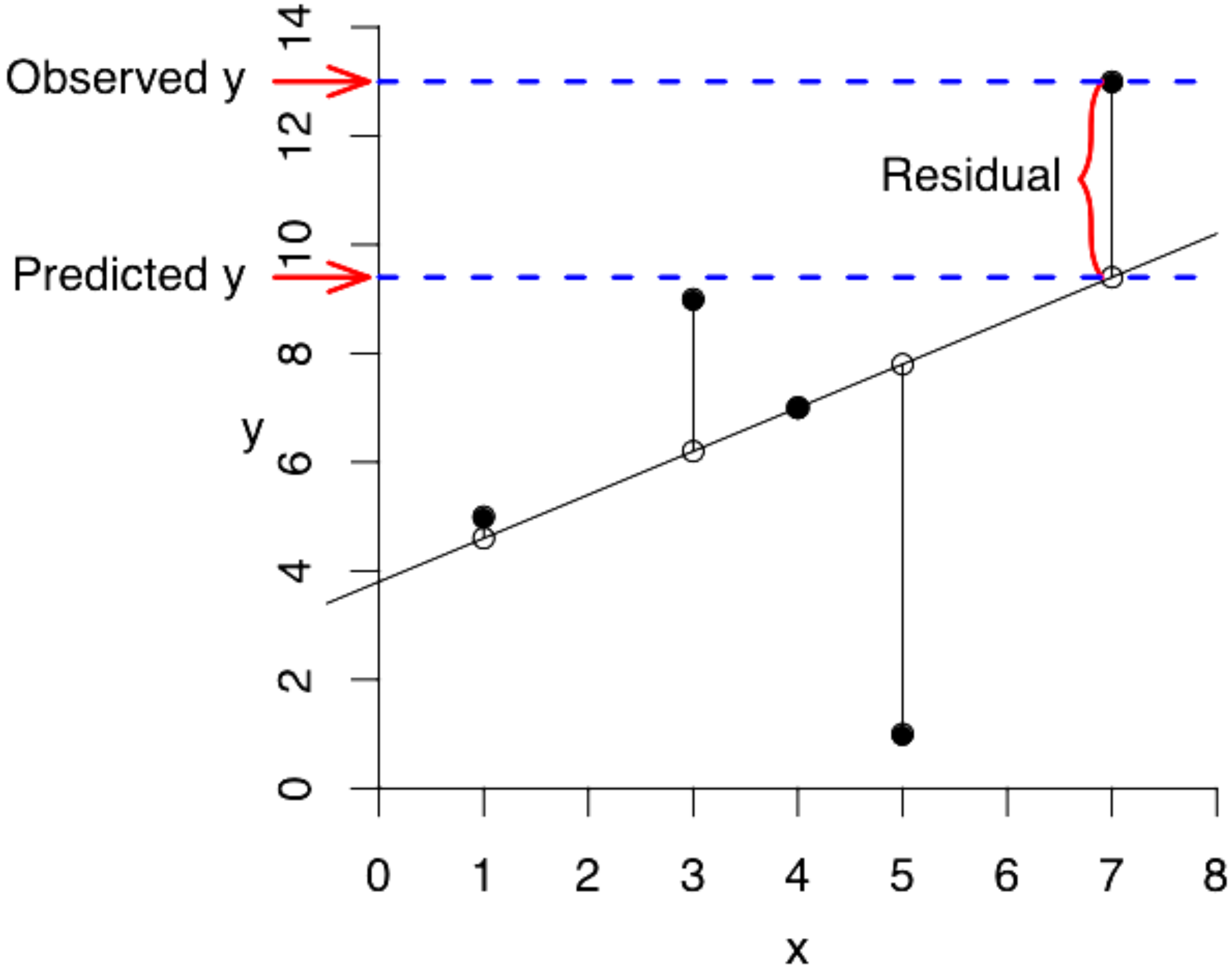
Root mean square

$$RMS = \sqrt{\frac{\Sigma\ (\hat{y}_i - yi\ )^2}{n}}$$

Summed absolute error

$$SAE = \Sigma\ |\hat{y}_i - y_i\ |$$

"Regression" = prediction of values



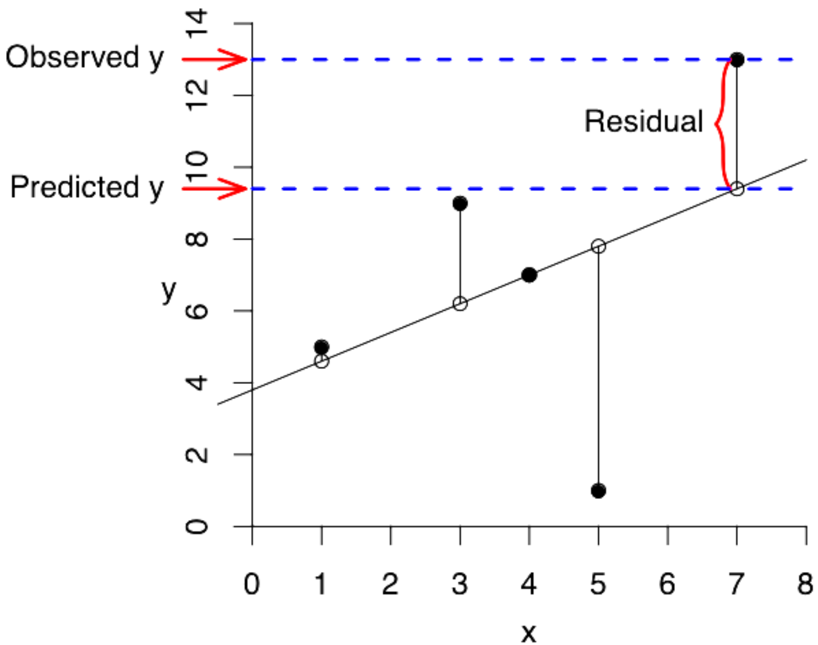
Summed squared error

$$SSE = \Sigma (\hat{y}_i - y_i)^2$$

Summed absolute error

$$SAE = \Sigma |\hat{y}_i - y_i|$$

I don't have to calculate these because of the argmin symmetries.
These are monotonic functions of SSE and SAE



Mean squared error

$$MSE = \frac{\Sigma\,(\hat{y}_i - yi\,)^2}{n}$$

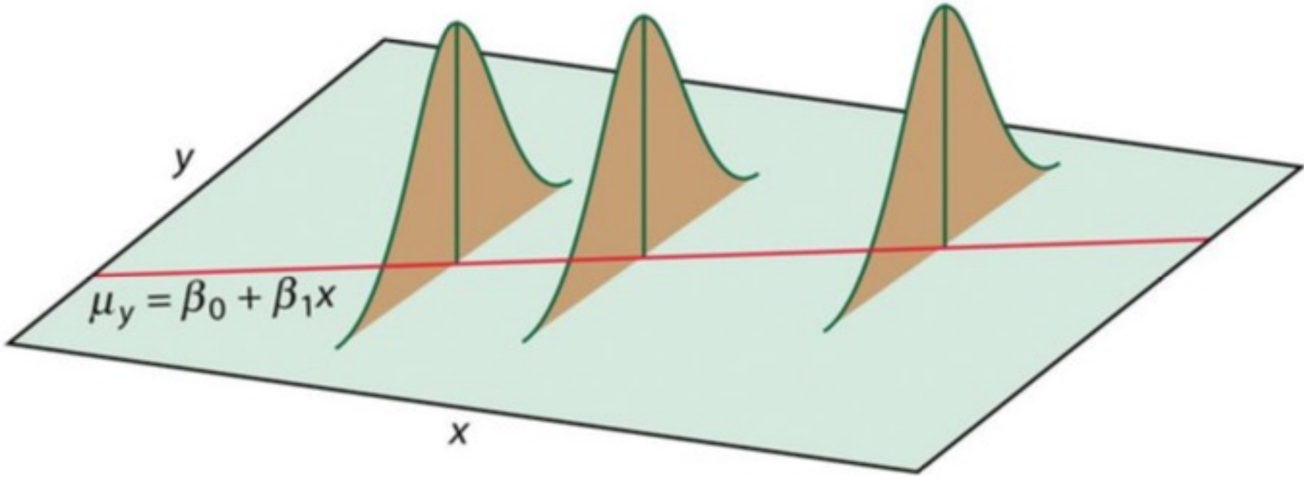
Root mean square

$$RMS = \sqrt{\frac{\Sigma\,(\hat{y}_i - yi\,)^2}{n}}$$

Mean absolute error

$$MAE = \frac{\Sigma\,|\hat{y}_i - yi|}{n}$$

Consequences of sum-squared-error



- Minimizing sum-squared error solves the problem of model + additive normally-distributed noise in y where **the noise level at each point is the same.**
- This is often not reasonable; each point often should not get the same weight. **Examples?**
- Weighted (per-datapoint) sums of sum-squared error relax this requirement if you have a theoretical (or empirical) reason to estimate them differently. (Standard error of the mean, anyone?)

Loss function sometimes implies probability

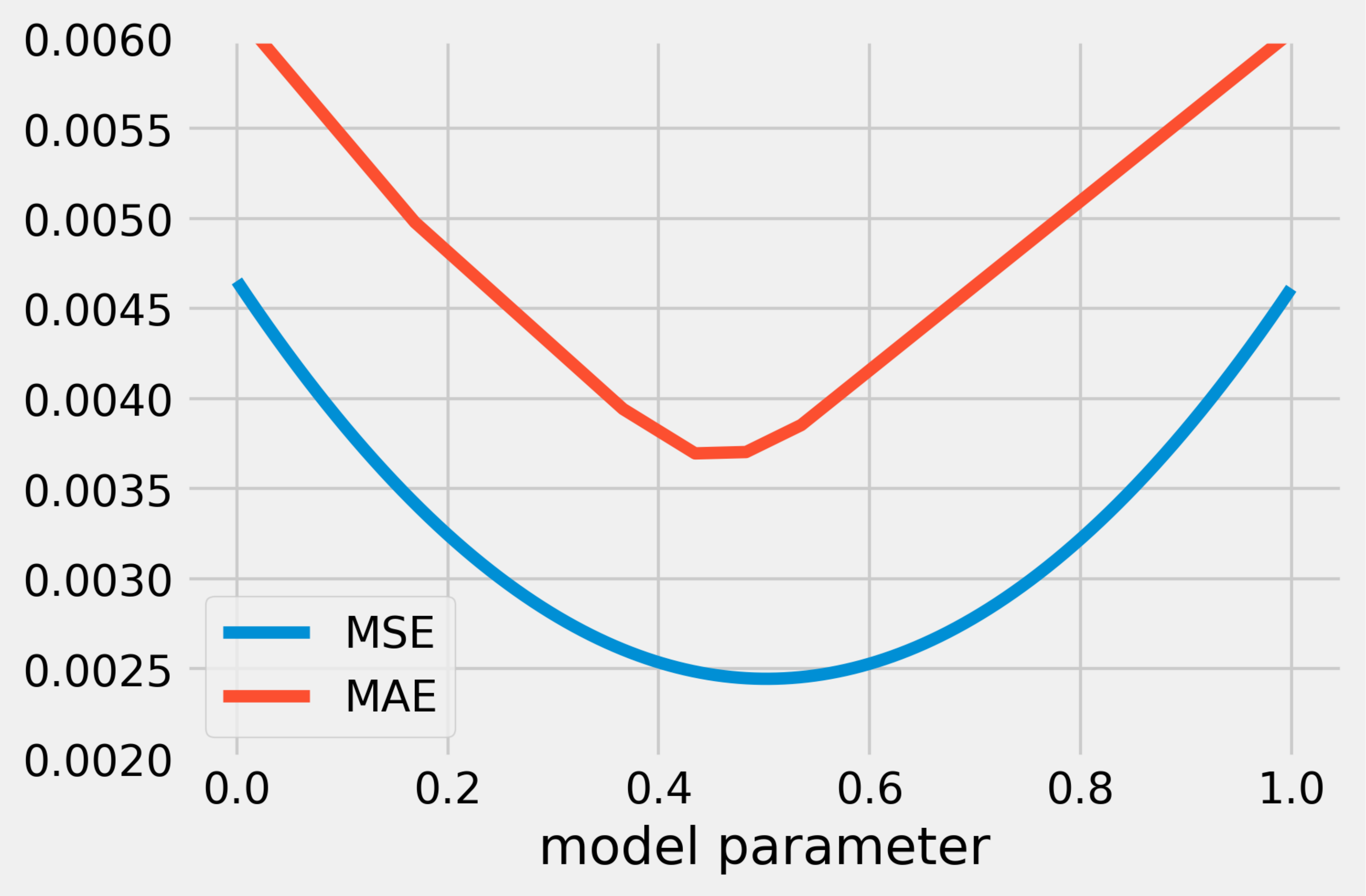
- When the objective function looks like (is proportional to) a log-probability function, optimizing it looks a lot like maximum likelihood / maximum a posteriori estimation.
- Sum squared errors.. are the log of additive normal error distributions
- Certain regularization terms , like $w^T w$, solve the problem with as if the total probability distribution includes normal priors on the components of w. (!!!)
- Nice if it’s bounded below
- Discontinuities are frowned upon.

Objective function options : choices

- The choice of function here sets the balance between small errors and large errors.

- Mean Squared Error / sum squared error "L2 loss function"
  - penalizes large errors much more than small ones
- Mean absolute error "L1 loss function"
  - discontinuous derivative; derivative does not vanish anywhere; all the points pull on the fit whether above or below the fit.
- Constraints on parameters, parameter domain…
- Cross entropy or expected – log (p)
  - Useful for completely blind density fitting

Contrast L2 and L1



Discontinuities in the slope of mean absolute error.

Not analytic, not smooth…

Derivative won't vanish anywhere

Threshold effect when

$$\frac{\partial L}{\partial \theta} < \alpha$$

Contrast L2 and L1

- L2 in the residuals gives the same solution as optimizing additive normally distributed errors.
- L1 in the residuals give the same solution as optimizing Laplace-distributed errors.
- But we can add terms to the loss function that don’t correspond to probability distributions.. these will steer the solution around..

Loss functions for categorical data:

- "Accuracy" -- number of correct assignments on the test set
- Makes sense to assign penalties to each wrong answer. They can be all the same or they can be different

CIFAR-10 Confusion Matrix

True Class \ Predicted Class	airplane	automobile	bird	cat	deer	dog	frog	horse	ship	truck		
airplane	923	4	21	8	4	1	5	5	23	6	92.3%	7.7%
automobile	5	972	2					1	5	15	97.2%	2.8%
bird	26	2	892	30	13	8	17	5	4	3	89.2%	10.8%
cat	12	4	32	826	24	48	30	12	5	7	82.6%	17.4%
deer	5	1	28	24	898	13	14	14	2	1	89.8%	10.2%
dog	7	2	28	111	18	801	13	17		3	80.1%	19.9%
frog	5		16	27	3	4	943	1	1		94.3%	5.7%
horse	9	1	14	13	22	17	3	915	2	4	91.5%	8.5%
ship	37	10	4	4		1	2	1	931	10	93.1%	6.9%
truck	20	39	3	3			2	1	9	923	92.3%	7.7%
	88.0%	93.9%	85.8%	79.0%	91.4%	89.7%	91.6%	94.1%	94.8%	95.0%		
	12.0%	6.1%	14.2%	21.0%	8.6%	10.3%	8.4%	5.9%	5.2%	5.0%		

Expected loss

For unknown state of nature P(ω_j | x) , and action α the risk associated with action α_i is the weighted sum of the loss function $\lambda(\alpha_i|\omega_j)$ over all the possible states of nature P(ω_j | x)

- $R(\alpha_i \mid \mathbf{x}) = \sum_j \lambda(\alpha_i \mid \omega_j) P(\omega_j \mid \mathbf{x})$

This means I need to define a loss $\lambda(\alpha_i|\omega_j)$ for every element of the confusion matrix.

Thoughts on the loss

- Perhaps a different value for λ (gorilla | human) than for

λ (dog | cat) for general-purpose images?

- At first glance, this looks like a place that we could fit our preferences for the balance between type-I and type-II errors.

- λ (no action | unexpected pedestrian walking in front of car)

- λ (take action so extreme it may cause injury | unexpected pedestrian walking in front of car)

Zero-one loss function

- The simplest loss function, called the zero-one loss function, is just zero for all of the correct decisions and one for all of the incorrect decisions.

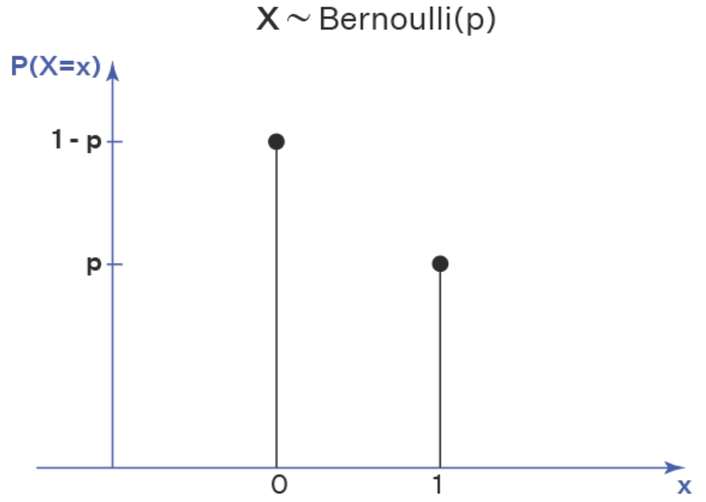
$$\lambda_{ij} = 1 - \delta(i, j)$$

This counts the number of errors.

$$\lambda = \begin{matrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{matrix}$$

How about the domains?

- When estimating probabilities (like mixing ratios) some parameters naturally live in the parameter space of the Bernoulli (or multinomial / categorical distribution)
- That is to say, there are a lot of useful parameters out there that are between 0 and 1.
- How do we search a space without running out of the domain?



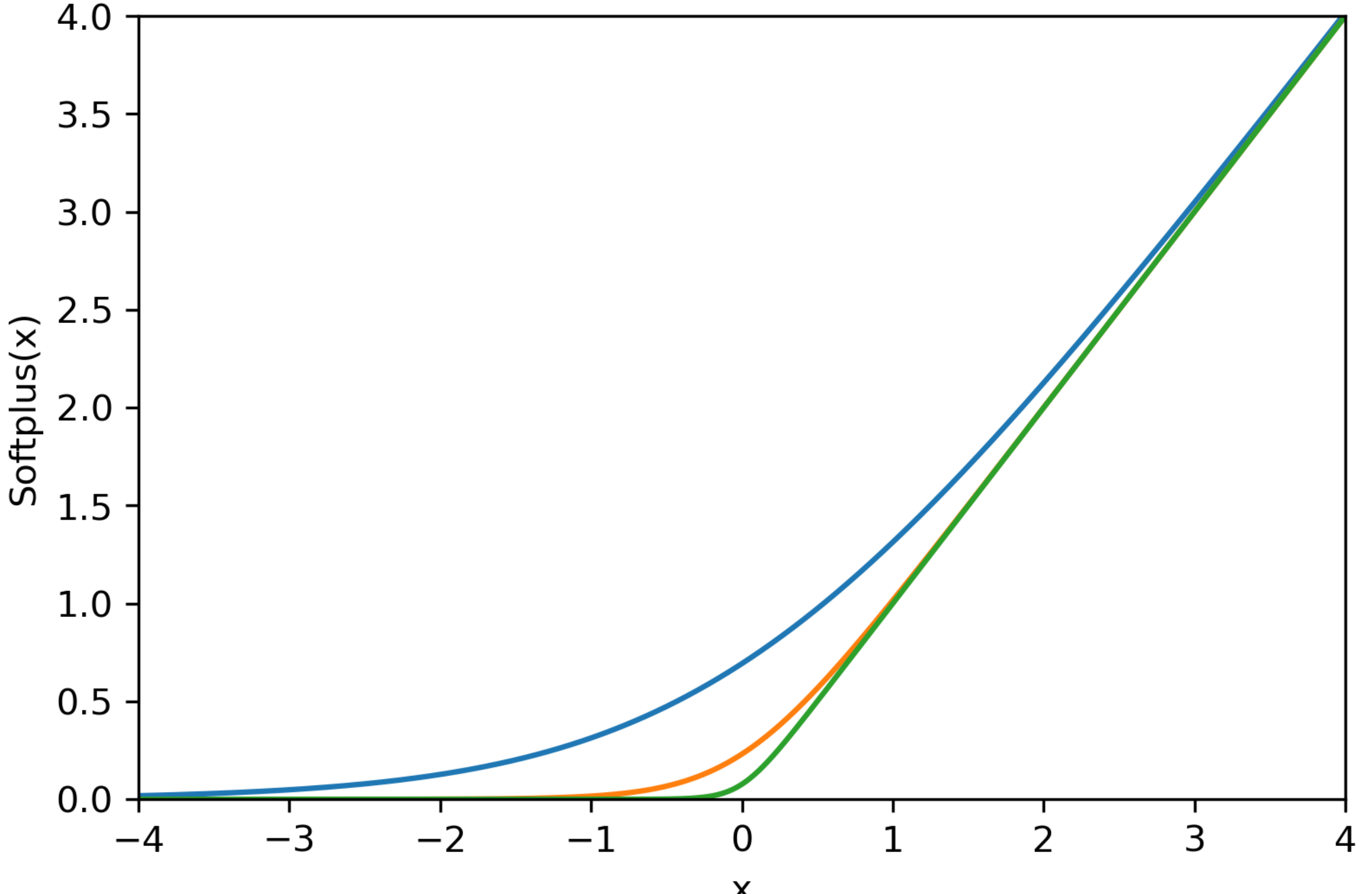
Loss (min(max(0, x), 1))   is not a good choice.

$\text{Loss}_{\text{CONSTRAINED}} = \text{Loss} + \text{HUGE} (x > 1) + \text{HUGE} (x < 0)$

also not a good choice

Softplus

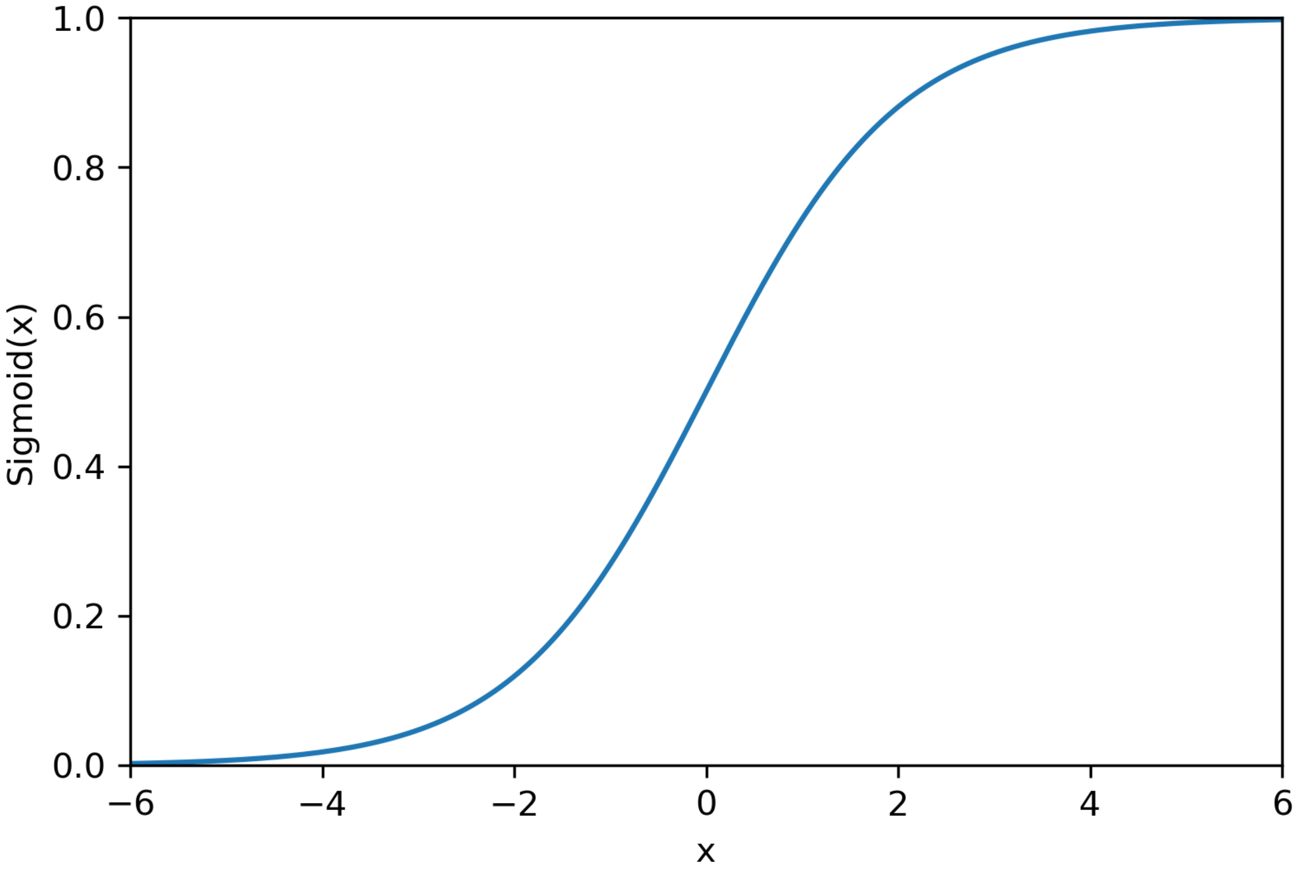
$$softplus(x) = \log(\, 1 + \exp(x))$$



- gentler form of max(0, x)

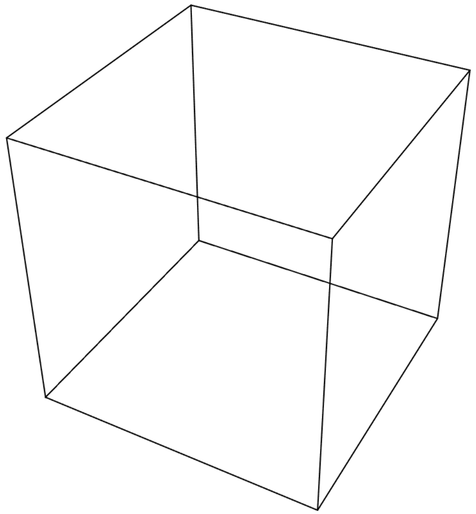
Sigmoid function

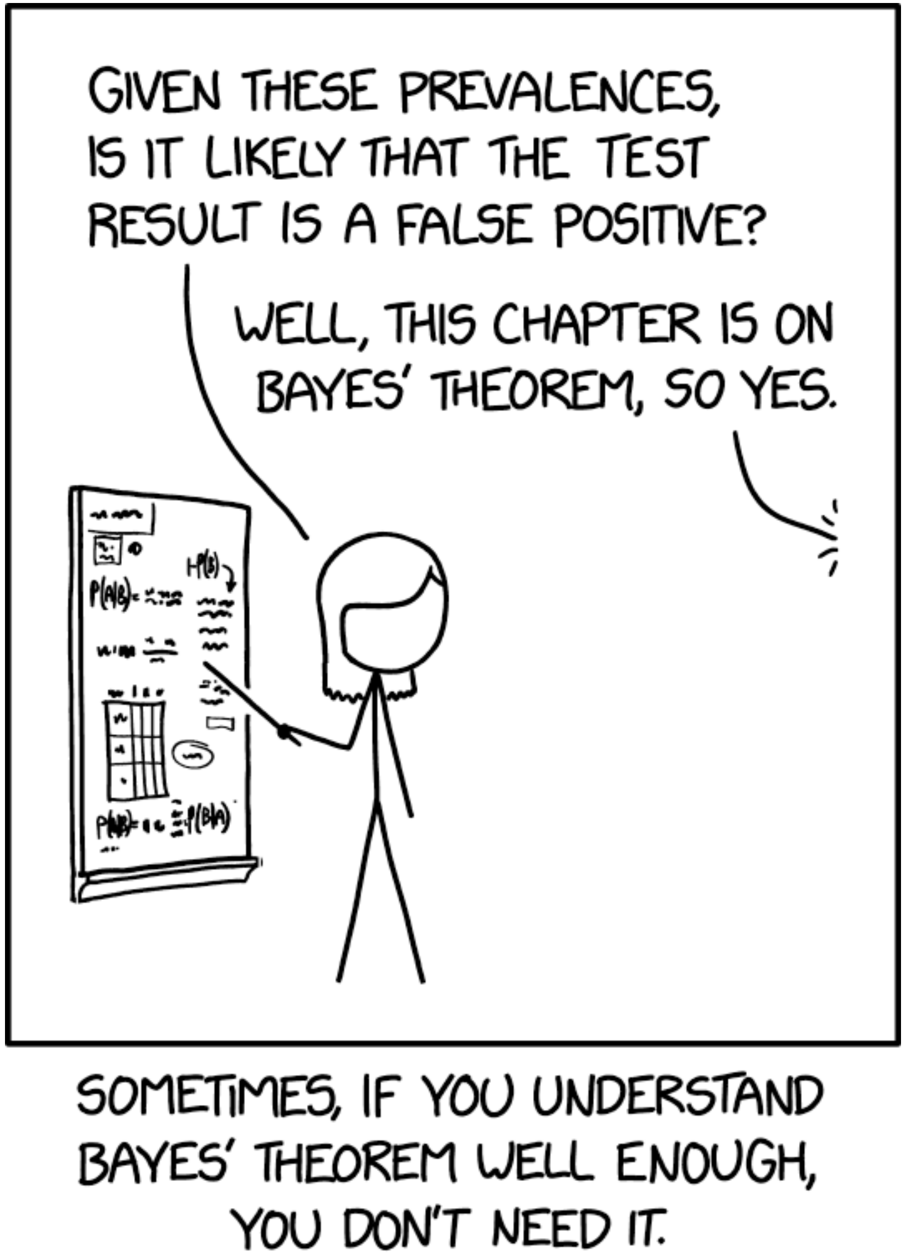
$$sigmoid(x) = \frac{\exp(x)}{1 + \exp(x)}$$



- gentler form of 0.5* sign(x) + 0.5
- continuous mapping from $\mathbb{R}$ to (0,1)

$\mathbb{R}^3$ -> 1^3





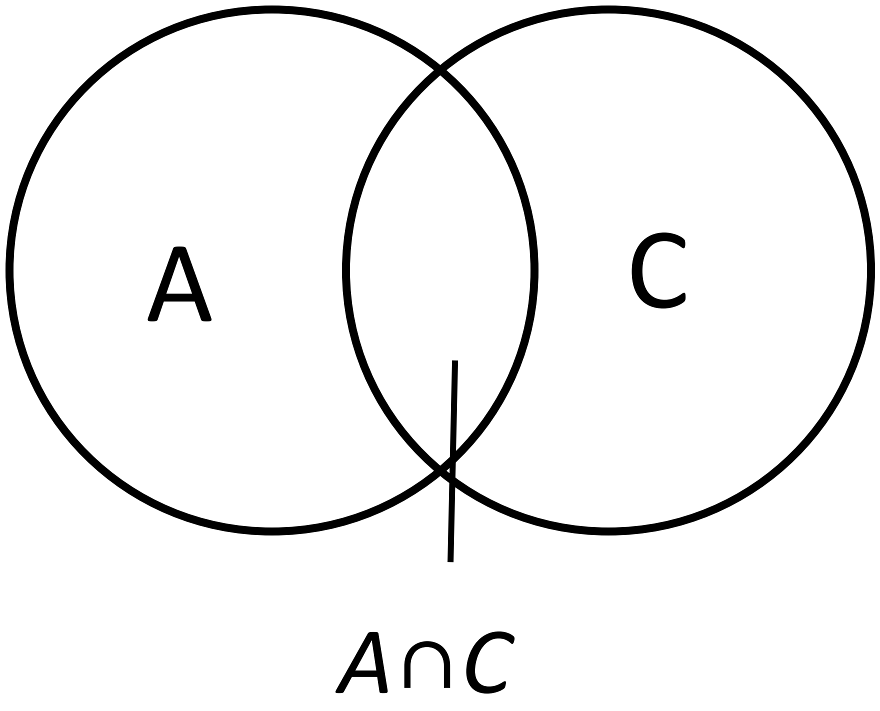
In favorable cases, we can use Bayes' theorem to estimate our parameters.

In less favorable cases, we can do a randomized search for possible parameter values.

Bayesian inference

Event A: unknown state of nature
Event C: experiment

$$P(A \mid C) = P(C|A)\,P(A) / P(C)$$



Bayesian inference

Event A: unknown state of nature

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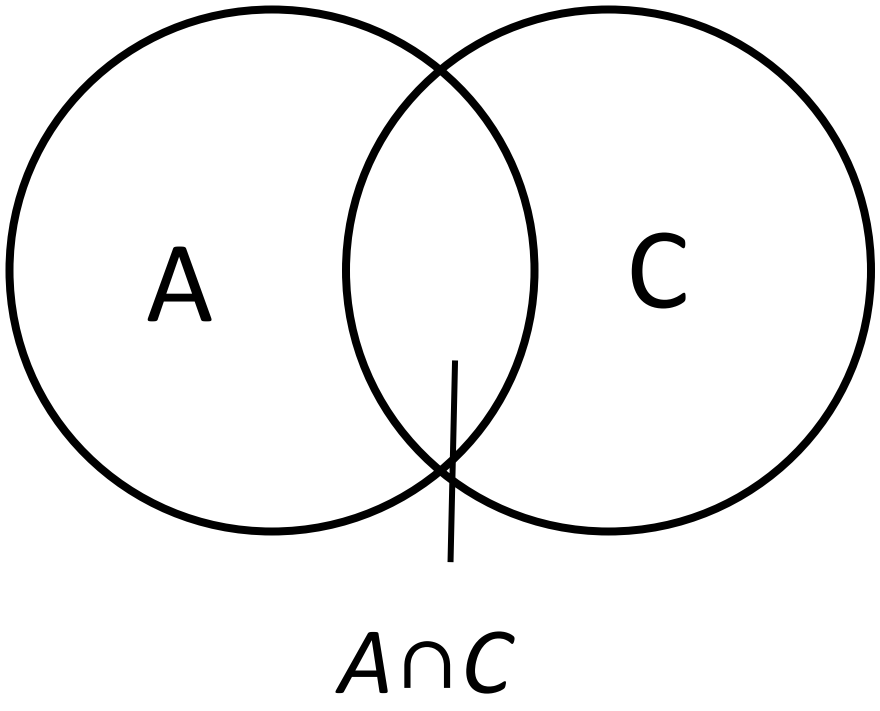


"Numerical decisionmaking for grownups"

Bayesian inference

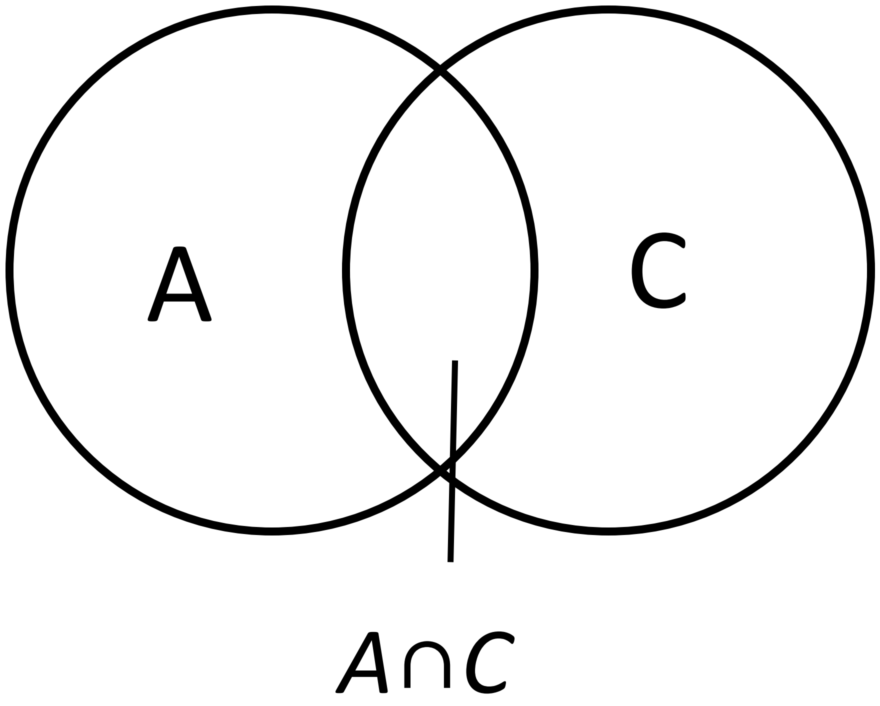
Event A: am I infected?

Event C: experiment (test result)

$$P(A \mid C) = P(C|A)\, P(A) / P(C)$$

The thing I want to know

The thing the FDA wants know



Bayesian inference

Event A: unknown state of nature

Event C: experiment

$$P(A \mid C) = P(C|A)\, P(A) \,/\, P(C)$$

Life's persistent question

Term that depends on experiment

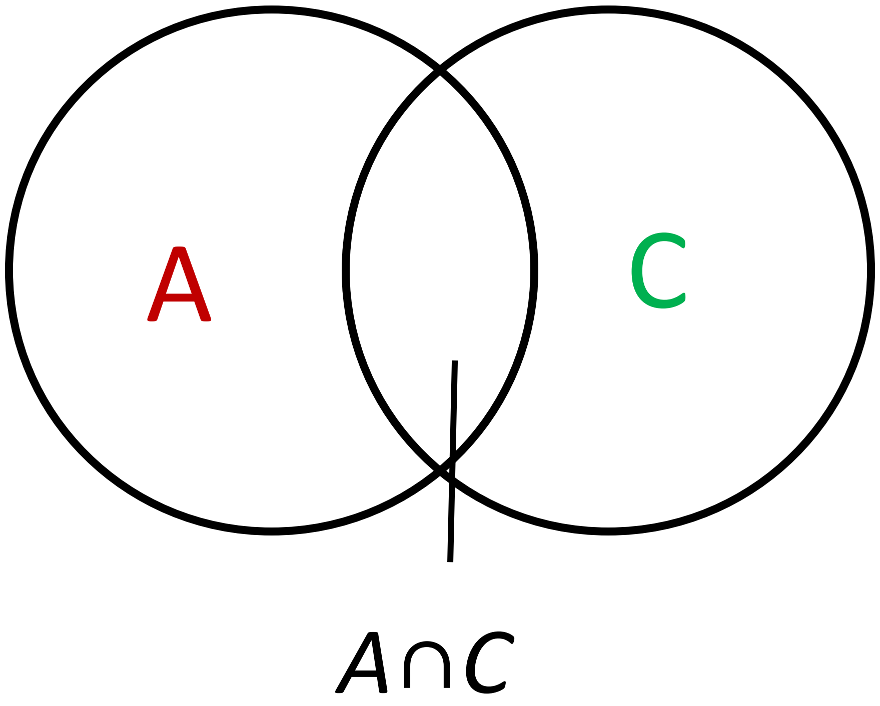
likelihood

Term with knowledge and bias about A

prior

Probability for event that is no longer uncertain

evidence



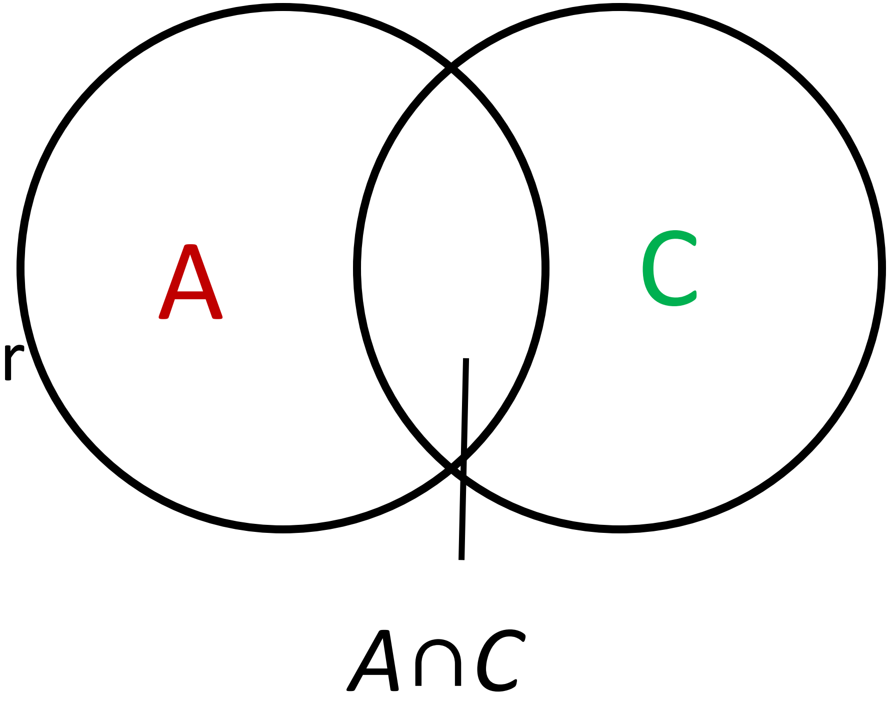
Bayesian inference

Event A: value of parameter

Event C: data

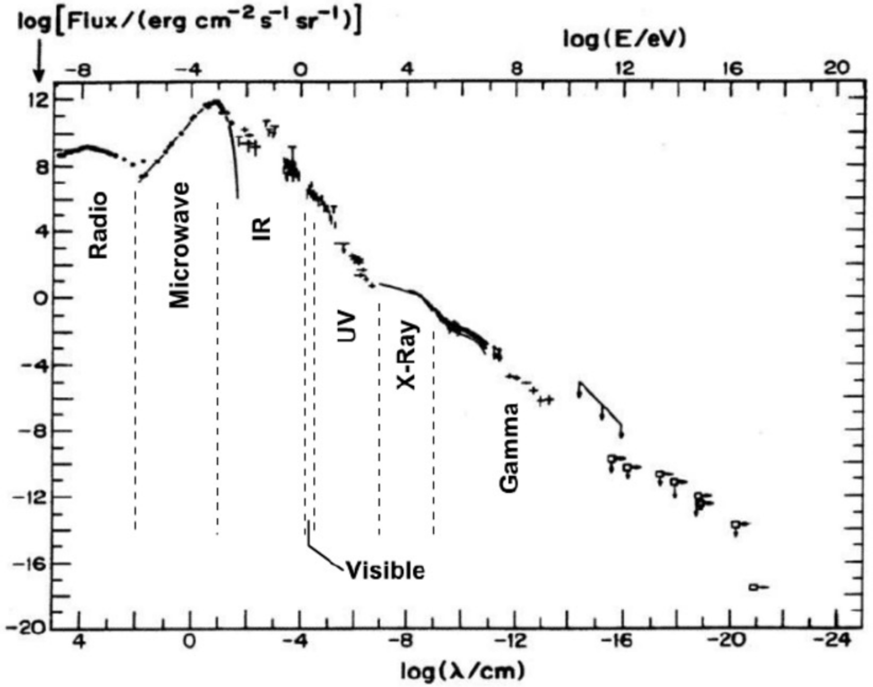
$$P(A \mid C) = P(C \mid A)\, P(A) \,/\, P(C)$$

Desired distribution/ parameter value	This is the	Prior distribution for parameter	Doesn't matter for us
posterior	*likelihood*	*prior*	*evidence*



Why do we take logs?

- Mathematical convenience; turns multiplication into addition
- Dynamic range; floating points only store 15 digits (Anyone tried to calculate 500 Choose 498 on a calculator?)
- Numerical precision: probabilities in high-dimensional space run into underflow problems
- log-transform is monotonic, so the location of the optimum is unperturbed



Log (Bayesian inference)

Event A: unknown parameter

Event C: data

$$\log P(A \mid C) = \log P(C|A) + \log P(A) - \log P(C)$$

Desired parameter distribution

The likelihood

likelihood

Prior distribution on the parameter

depends only on the data

posterior

likelihood

prior

evidence

Bayesian inference

θ: value of parameter

Y: data

$$P(\theta \mid Y) = P(Y \mid \theta)\, P(\theta) \,/\, P(Y)$$

Distribution to help me find the parameter value

posterior

This is the likelihood

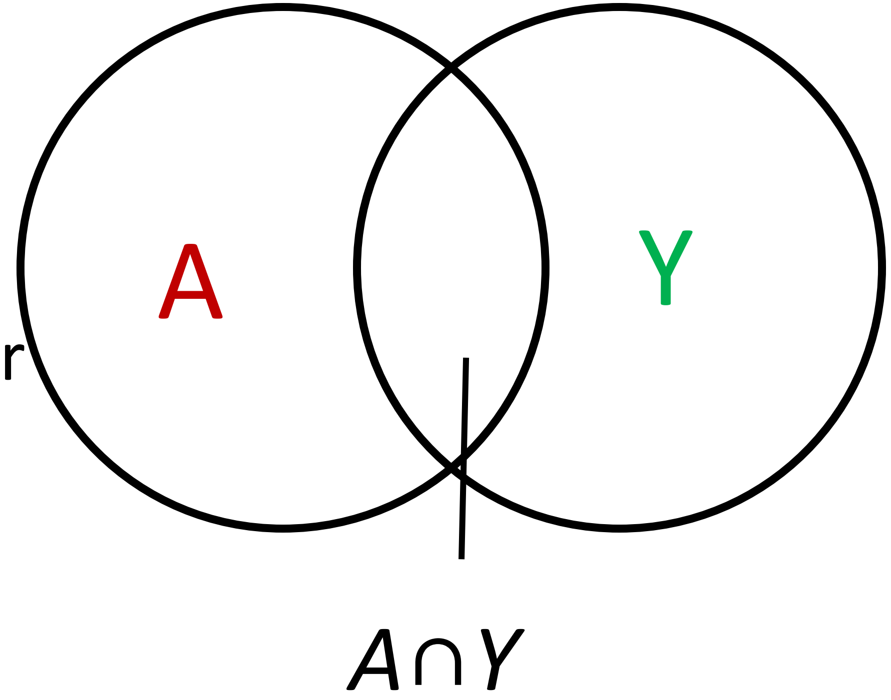
likelihood

Prior distribution for parameter

prior

Doesn't matter for us

evidence



Bayesian inference for sequential

θ: value of parameter

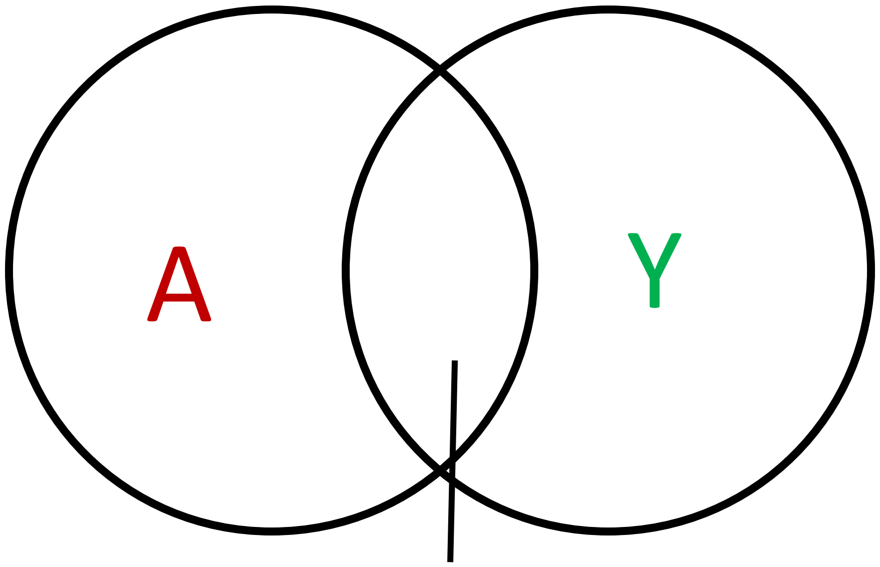
Y: data

$$P(\theta \mid \{Y_i\}) = \Pi P_i(Y|\theta)\, P(\theta)$$

Posterior density

Product of likelihoods of independent observations

One factor of the prior on the parameter



$A \cap Y$

posterior

likelihood

prior

Where does the prior come from?

- In some cases, there will be a correspondence between our objective function and the solution to a Bayesian inference problem.
- If we were doing this the other way, taking inference as our approach to problem-solving, we would choose prior distributions either from
  - Prior research into the values of the parameters (common in physical sciences)
  - Symmetries of the problem (geometry) that makes certain classes of solution equivalent to certain other classes of solution.
- Some of these priors don't have finite integrals… "improper priors" usually the likelihood forces the product to converge; if it doesn't, we have to take the limit of a ratio of divergent integrals.
- Sometimes, the priors are chosen because they are easy to calculate

(good and bad)

Choices

- Location parameters (translational invariance) suggest uniform or "flat" priors. (Super easy ! just add dx !)
- Scale parameters that act by multiplication suggest priors proportional to $\frac{d\lambda}{\lambda}$. (But wait, doesn't that diverge? Yes. But the posterior shouldn't, unless the data fail to constrain your parameter.)
- Problems with rotational symmetry suggest priors for, for instance slope parameters, with uniform arctangents.
- Some problems (related to sampling) have prior distributions that are closely connected to the sampling process; these priors have the same form (but with different parameters) as the posteriors. These are called **conjugate priors**

Homework guidelines

- No particular tools are required (python, R, javascript..) but we're better able to help you in python and R.
- Graphs are expected to a medium-high standard. Labels, units everywhere where needed. Caption-like explanations of graphs preferred.
- Upload PDFs of answers to Canvas. Separately upload code (to a low standard) that you used to solve the homework. We probably won't look at the code.