Probabilistic Model Construction

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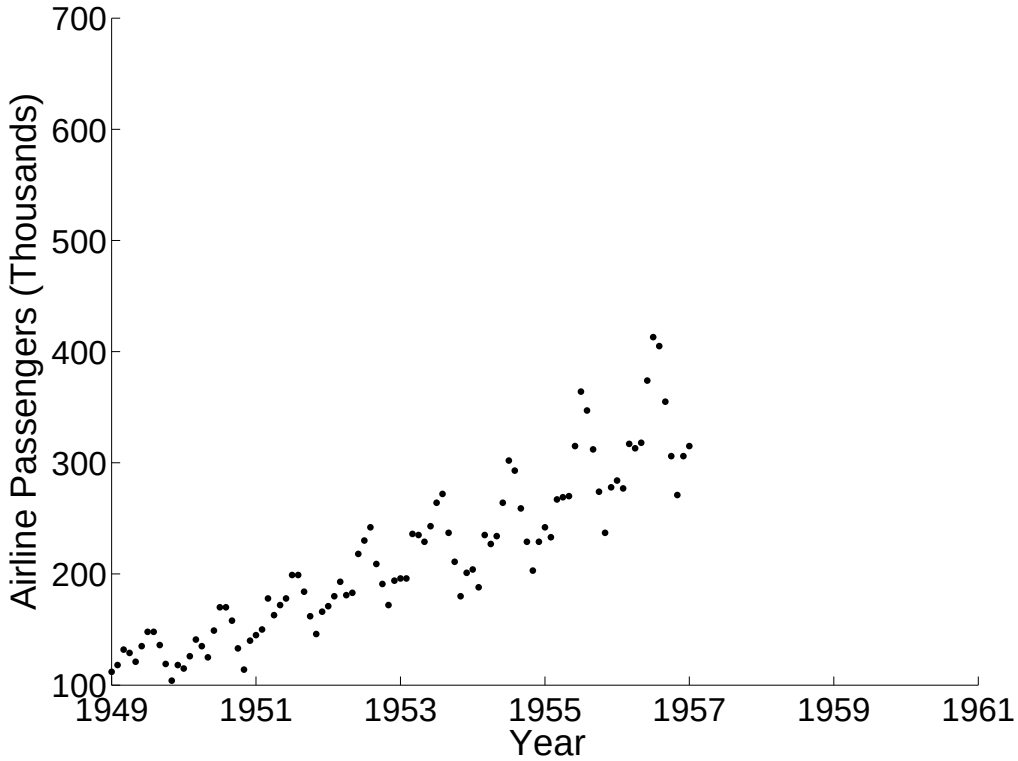
Model Selection



Which model should we choose?

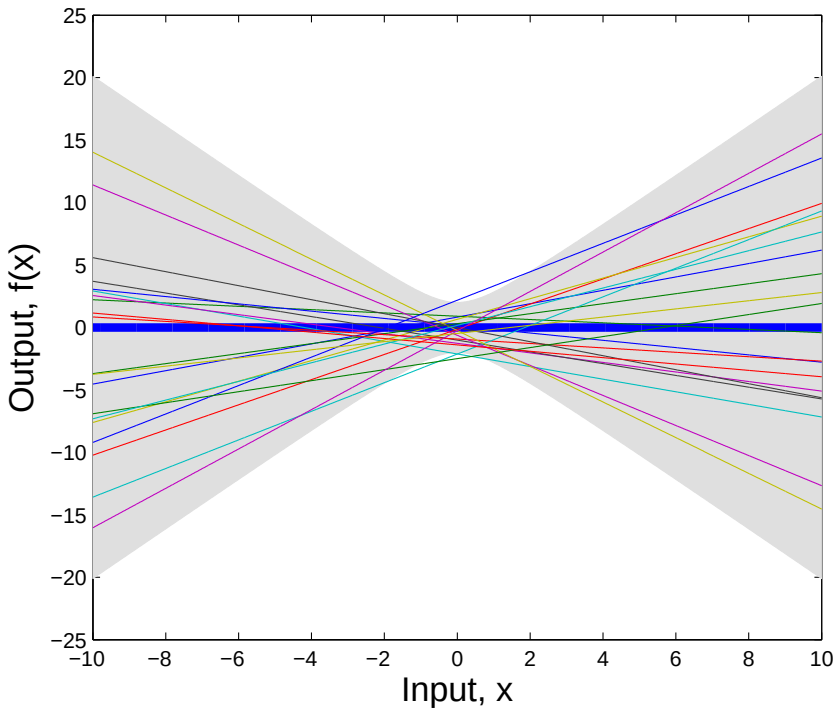
(1): $f_1(x) = w_0 + w_1 x$ **(2):** $f_2(x) = \sum_{j=0}^{3} w_j x^j$ **(3):** $f_3(x) = \sum_{j=0}^{10^4} w_j x^j$

A Function-Space View

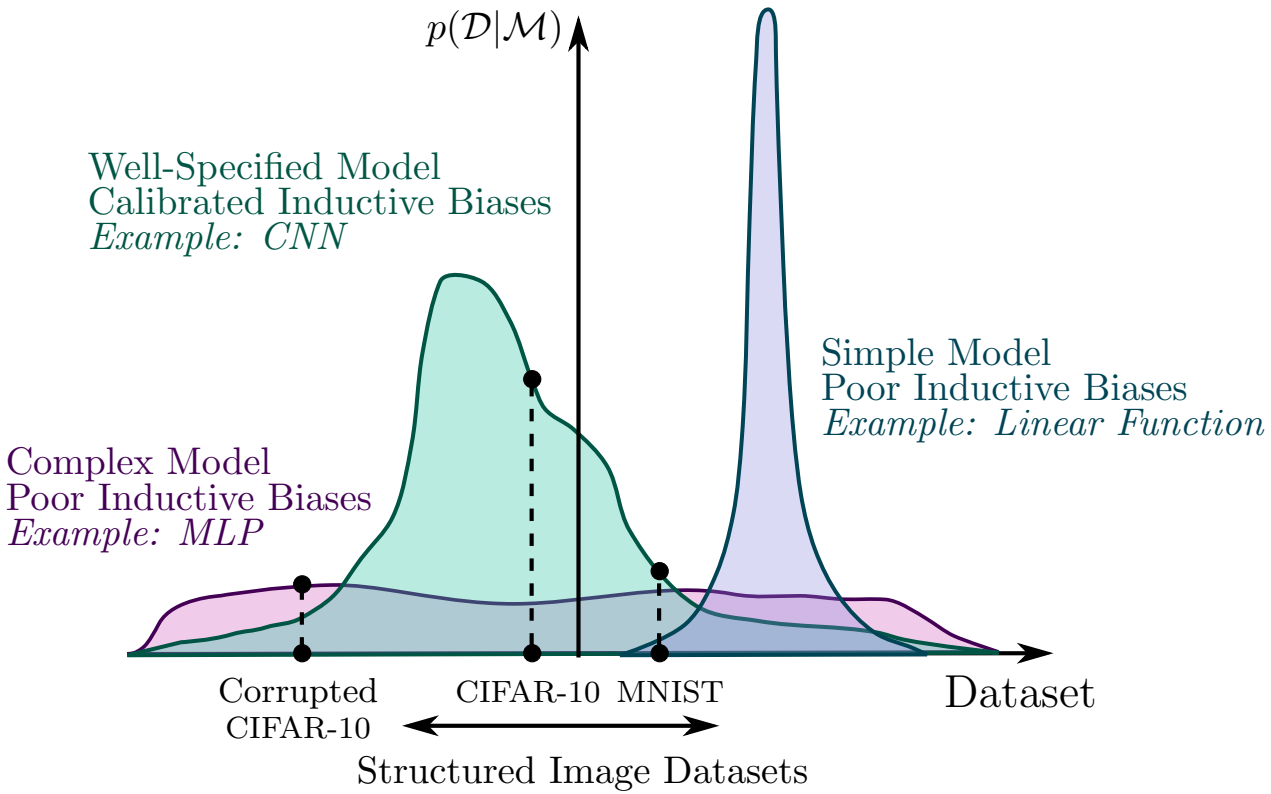
Consider the simple linear model,

$$f(x) = w_0 + w_1 x\,, \tag{1}$$

$$w_0, w_1 \sim \mathcal{N}(0, 1)\,. \tag{2}$$

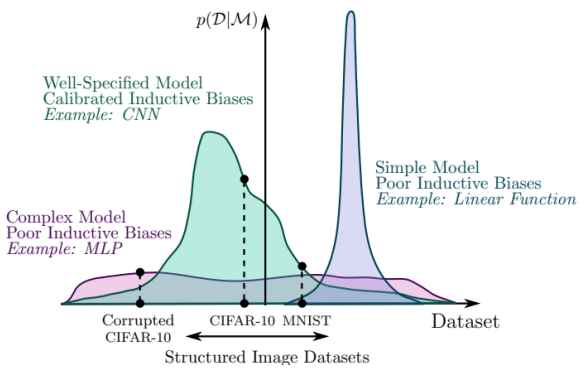


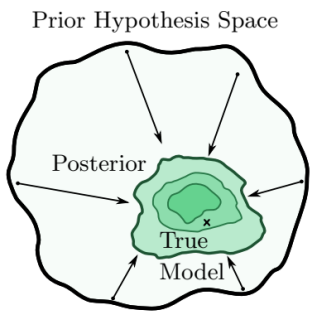
Model Construction and Generalization

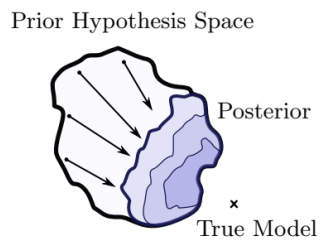


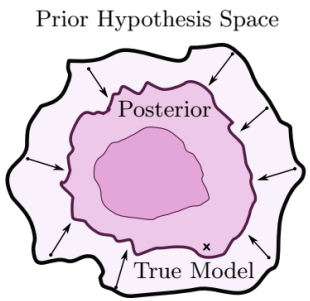
How do we learn?

- The ability for a system to learn is determined by its *support* (which solutions are a priori possible) and *inductive biases* (which solutions are a priori likely).
- We should not conflate *flexibility* and *complexity*.
- An influx of new *massive* datasets provide great opportunities to automatically learn rich statistical structure, leading to new scientific discoveries.





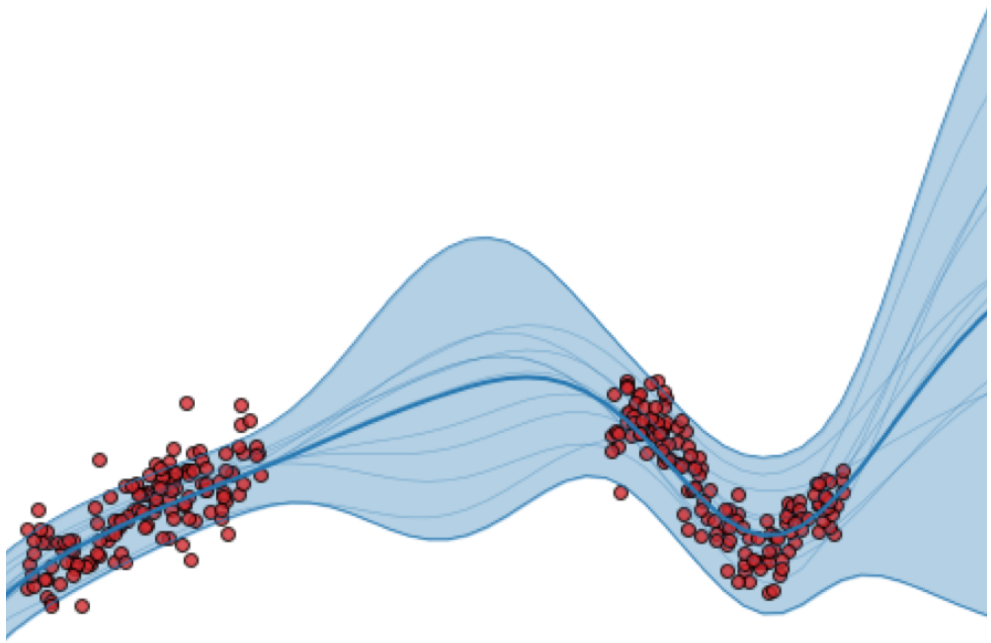


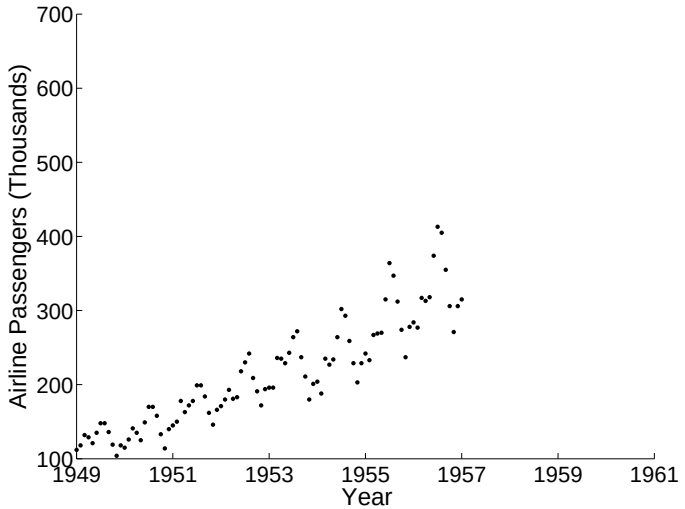


Bayesian Deep Learning and a Probabilistic Perspective of Generalization
Wilson and Izmailov, 2020
arXiv 2002.08791

What is Bayesian learning?

- The key distinguishing property of a Bayesian approach is **marginalization** instead of optimization.
- Rather than use a single setting of parameters **w**, use all settings weighted by their posterior probabilities in a *Bayesian model average*.





Basic Regression Problem

- Training set of n targets (observations) $\mathbf{y} = (y(x_1), \ldots, y(x_n))^{\mathrm{T}}$.
- Observations evaluated at inputs $X = (x_1, \ldots, x_n)^{\mathrm{T}}$.
- Want to predict the value of $y(x_*)$ at a test input x_*.

For example: Given airline passenger numbers $\mathbf{y}$ measured at times X, what will be the number of passengers when $x_* = 1961$?

Just knowing high school math, what might you try?

Guess the parametric form of a function that could fit the data

- $f(x, \mathbf{w}) = \mathbf{w}^{\mathrm{T}} x$ [Linear function of $\mathbf{w}$ and x]
- $f(x, \mathbf{w}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(x)$ [Linear function of $\mathbf{w}$] (Linear Basis Function Model)
- $f(x, \mathbf{w}) = g(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(x))$ [Non-linear in x and $\mathbf{w}$] (E.g., Neural Network)

$\boldsymbol{\phi}(x)$ is a vector of basis functions. For example, if $\boldsymbol{\phi}(x) = (1, x, x^2)$ and $x \in \mathbb{R}^1$ then $f(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2$ is a quadratic function.

Choose an error measure $E(\mathbf{w})$, minimize with respect to $\mathbf{w}$

- $E(\mathbf{w}) = \sum_{i=1}^{n} [f(x_i, \mathbf{w}) - y(x_i)]^2$

A probabilistic approach

We could explicitly account for noise in our model.

- $y(x) = f(x, \mathbf{w}) + \epsilon(x)$, where $\epsilon(x)$ is a noise function.

One commonly takes $\epsilon(x) = \mathcal{N}(0, \sigma^2)$ for i.i.d. additive Gaussian noise, in which case

$$p(y(x)|x, \mathbf{w}, \sigma^2) = \mathcal{N}(y(x); f(x, \mathbf{w}), \sigma^2) \qquad \text{Observation Model} \qquad (3)$$

$$p(\mathbf{y}|x, \mathbf{w}, \sigma^2) = \prod_{i=1}^{n} \mathcal{N}(y(x_i); f(x_i, \mathbf{w}), \sigma^2) \qquad \text{Likelihood} \qquad (4)$$

- Maximize the likelihood of the data $p(\mathbf{y}|x, \mathbf{w}, \sigma^2)$ with respect to $\sigma^2, \mathbf{w}$.

For a Gaussian noise model, this approach will make the same predictions as using a squared loss error function:

$$\log p(\mathbf{y}|X, \mathbf{w}, \sigma^2) \propto -\frac{1}{2\sigma^2} \sum_{i=1}^{n} [f(x_i, \mathbf{w}) - y(x_i)]^2 \qquad (5)$$

- The probabilistic approach helps us interpret the error measure in a deterministic approach, and gives us a sense of the noise level σ^2.
- Both approaches are prone to *over-fitting* for flexible $f(x, \mathbf{w})$: low error on the training data, high error on the test set.

Regularization

- Use a penalized log likelihood (or error function), such as

$$E(\mathbf{w}) = \overbrace{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(f(x_i,\mathbf{w}) - y(x_i)^2)}^{\text{model fit}} \overbrace{-\lambda \mathbf{w}^{\mathrm{T}}\mathbf{w}}^{\text{complexity penalty}} \quad . \tag{6}$$

- **But how should we define and penalize complexity?**
- Can set λ using *cross-validation*.
- Same as maximizing a posterior $\log p(\mathbf{w}|\mathbf{y}, X) = \log p(\mathbf{y}|\mathbf{w}, X) + \log p(\mathbf{w}) + c$ with a Gaussian prior $p(\mathbf{w})$. **But this is not Bayesian!**

Bayesian Inference

Bayes' Rule

$$p(a|b) = p(b|a)p(a)/p(b)\,, \qquad p(a|b) \propto p(b|a)p(a)\,. \tag{7}$$

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}, \quad p(\mathbf{w}|\mathbf{y}, X, \sigma^2) = \frac{p(\mathbf{y}|X, \mathbf{w}, \sigma^2)p(\mathbf{w})}{p(\mathbf{y}|X, \sigma^2)}\,. \tag{8}$$

Sum Rule

$$p(x) = \sum_y p(x, y) \tag{9}$$

Product Rule

$$p(x, y) = p(x|y)p(y) = p(y|x)p(x) \tag{10}$$

Bayesian Predictive Distribution

Sum rule: $p(x) = \sum_x p(x, y)$. **Product rule:** $p(x, y) = p(x|y)p(y) = p(y|x)p(x)$.

$$p(y|x_*, \mathbf{y}, X) = \int p(y|x_*, \mathbf{w})p(\mathbf{w}|\mathbf{y}, X)d\mathbf{w}\,. \tag{11}$$

- Think of each setting of $\mathbf{w}$ as a different model. Eq. (32) is a *Bayesian model average*, an average of infinitely many models weighted by their posterior probabilities.
- Represents *epistemic uncertainty* over which $f(x, w)$ fits the data.
- Automatically calibrated complexity even with highly flexible models.
- Can view classical training as using an approximate posterior $q(\mathbf{w}|\mathbf{y}, X) = \delta(w = w_{\text{MAP}})$.

Bayesian Model Averaging is Not Model Combination

$$p(y|\mathcal{D}) = \sum_h p(y|h)p(h|\mathcal{D})$$

- The weights $p(h|\mathcal{D})$ only represent a statistical inability to distinguish between hypotheses.
- Assumes that combination models are not in the hypothesis space.
- In the limit of infinite data, $p(h|\mathcal{D})$ will collapse onto a point mass.

Bayesian model averaging is not model combination. Minka, T. Technical Report, 2000.

Example: Biased Coin

Suppose we flip a biased coin with probability λ of landing tails.

1. What is the likelihood of a set of data $\mathcal{D} = \{y_1, y_2, \ldots, y_n\}$?
2. What is the maximum likelihood solution for λ?
3. Suppose the first flip is tails. What is the probability that the next flip will be a tails, using maximum likelihood?

Example: Biased Coin

Likelihood of the data:

$$p(\{y_i\}_{i=1}^n) = \prod_{i=1}^{n} \lambda^{y_i}(1-\lambda)^{1-y_i} \tag{12}$$

where $y_i = 1$ if y_i is tails, and $y_i = 0$ if y_i is heads.

Likelihood of getting m tails is

$$p(\mathcal{D}|m,\lambda) = \binom{n}{m}\lambda^m(1-\lambda)^{n-m} \tag{13}$$

Example: Biased Coin

Likelihood of getting m tails is

$$p(\mathcal{D}|m,\lambda) = \binom{n}{m}\lambda^m(1-\lambda)^{n-m} \tag{14}$$

The maximum likelihood solution is

$$\hat{\lambda}_{\mathrm{ML}} = \mathrm{argmax}_\lambda p(\mathcal{D}|m,\lambda) = \frac{m}{n} \tag{15}$$

Example: Biased Coin

Likelihood of getting m tails is

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The maximum likelihood solution is

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Do you believe this solution? Why or why not?

Example: Biased Coin

Likelihood of getting m tails is

$$p(\mathcal{D}|m,\lambda) = \binom{n}{m}\lambda^m(1-\lambda)^{n-m} \tag{18}$$

Example: Biased Coin

Likelihood of getting m tails is

$$p(\mathcal{D}|m,\lambda) = \binom{n}{m}\lambda^m(1-\lambda)^{n-m} \tag{19}$$

If we choose a prior $p(\lambda) \propto \lambda^\alpha(1-\lambda)^\beta$ then the posterior will have the same functional form as the prior.

Example: Biased Coin

Likelihood of getting m tails is

$$p(\mathcal{D}|m,\lambda) = \binom{n}{m}\lambda^m(1-\lambda)^{n-m} \tag{20}$$

If we choose a prior $p(\lambda) \propto \lambda^\alpha(1-\lambda)^\beta$ then the posterior will have the same functional form as the prior.
We can choose the beta distribution:

$$Beta(\lambda|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\lambda^{a-1}(1-\lambda)^{b-1} \tag{21}$$

The Gamma functions ensure that the distribution is normalized:

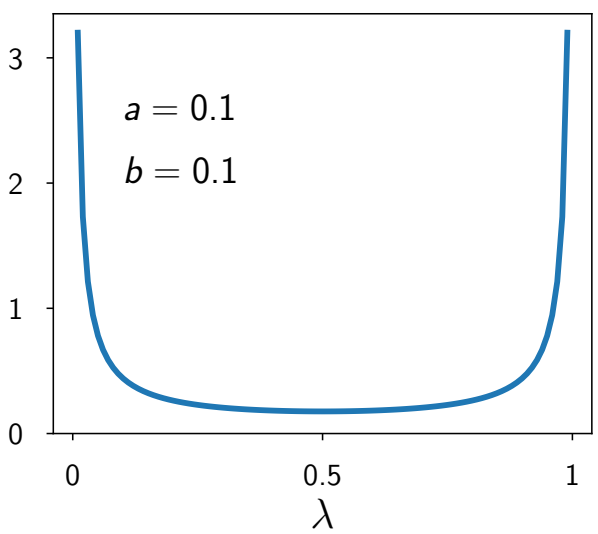
$$\int Beta(\lambda|a,b)d\lambda = 1 \tag{22}$$

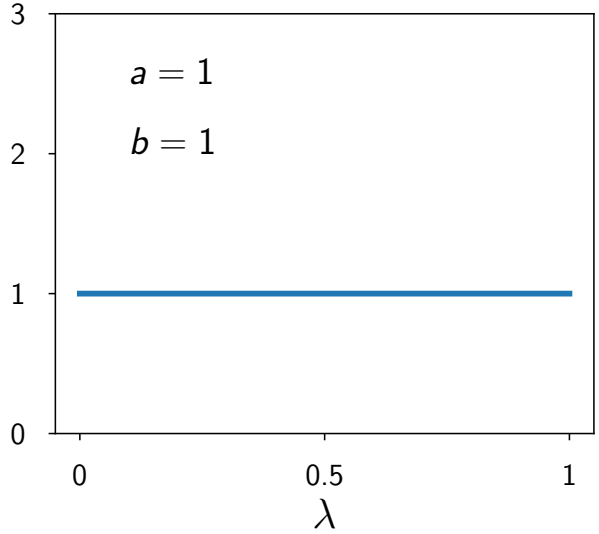
Moments:

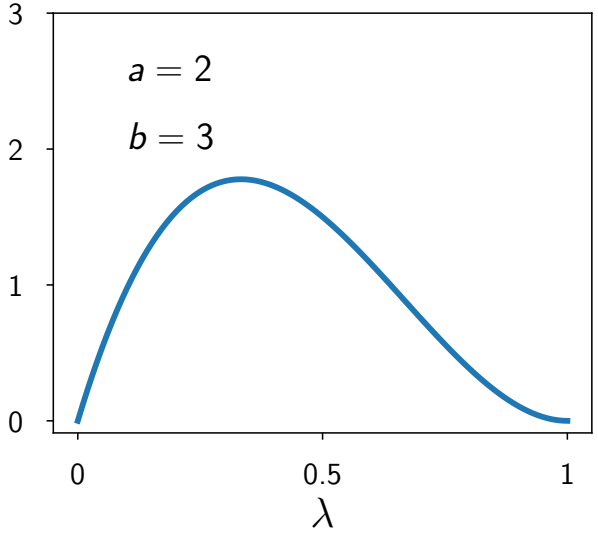
$$\mathbb{E}[\lambda] = \frac{a}{a+b} \tag{23}$$

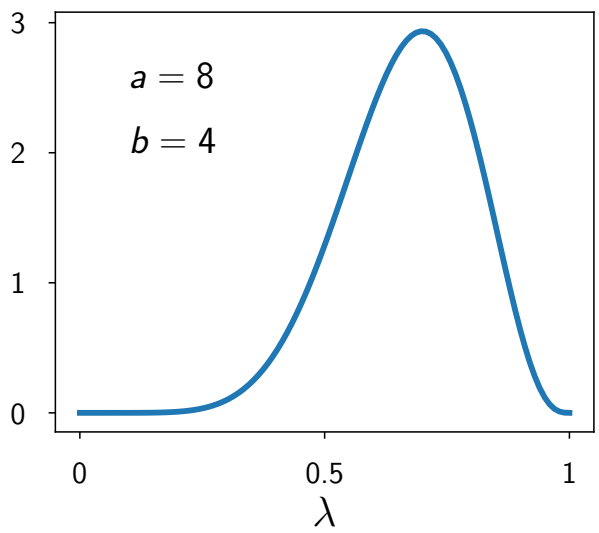
$$\text{var}[\lambda] = \frac{ab}{(a+b)^2(a+b-1)}\,. \tag{24}$$

Beta Distribution

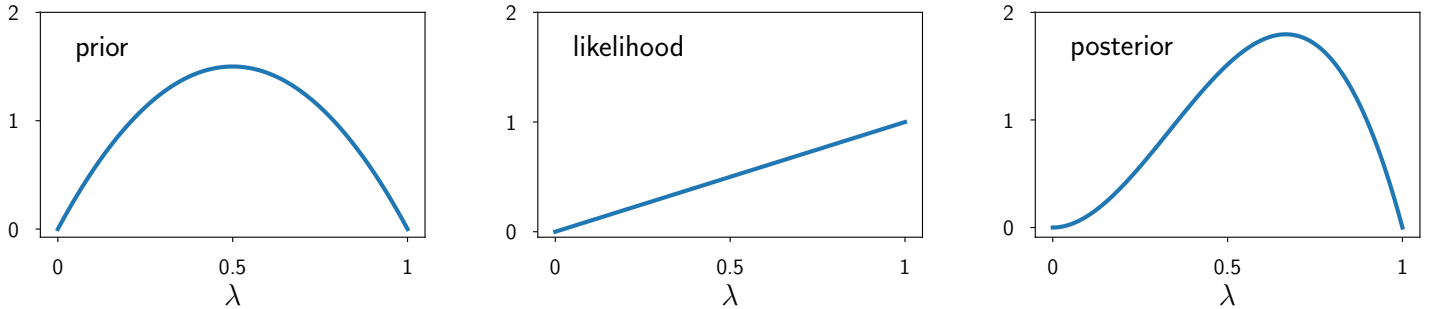








Example: Biased Coin



Applying Bayes theorem, we find:

$$p(\lambda|\mathcal{D}) \propto p(\mathcal{D}|\lambda)p(\lambda) \tag{25}$$

$$= Beta(\lambda; m+a, n-m+b) \tag{26}$$

We can view a and b as pseudo-observations!

$$\mathbb{E}[\lambda|\mathcal{D}] = \frac{m+a}{n+a+b} \tag{27}$$

1. What is the probability that the next flip is tails?
2. What happens in the limits of a, b?
3. What happens in the limit of infinite data?

Example: Biased Coin

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$$p(\lambda|\mathcal{D}) \propto p(\mathcal{D}|\lambda)p(\lambda) \tag{28}$$

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$$\mathbb{E}[\lambda|\mathcal{D}] = \frac{m+a}{n+a+b} \tag{30}$$

1. What is the probability that the next flip is tails?
2. What happens in the limits of a, b?
3. What happens in the limit of infinite data?
4. **Does the MAP estimate**

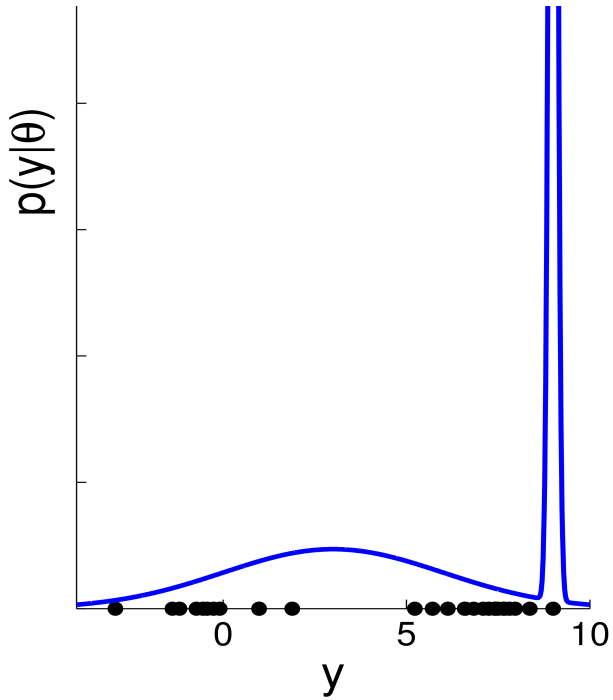
$$\hat{\lambda}_{MAP} = \textbf{argmax}_\lambda \log p(\lambda|\mathcal{D}) = \textbf{argmax}_\lambda \log p(\mathcal{D}|\lambda) + \log p(\lambda) \tag{31}$$

with a uniform prior $p(\lambda)$ give the same answer as Bayesian marginalization to find $p(\text{tails next flip}|\mathcal{D}) = \int \lambda p(\lambda|\mathcal{D})d\lambda = \mathbb{E}[\lambda|\mathcal{D}]$ with a uniform prior $p(\lambda)$?

Example: Density Estimation

- Observations $y_1, \ldots, y_n$ from unknown density $p(y)$.
- Specify an observation model. For example, we can let the points be drawn from a mixture of Gaussians:
  $p(y|\theta) = w_1 \mathcal{N}(y|\mu_1, \sigma_1^2) + w_2 \mathcal{N}(y|\mu_2, \sigma_2^2)$,
  $\theta = \{w_1, w_2, \mu_1, \mu_2, \sigma_1, \sigma_2\}$.
- Likelihood $p(\mathbf{y}|\theta) = \prod_{i=1}^{n} p(y_i|\theta)$.

Can learn all free parameters θ using maximum likelihood...



$$\hat{\theta}_{\mathrm{ML}} = \mathrm{argmax}_\theta \prod_{i=1}^{n} \frac{w_1}{\sqrt{2\pi\sigma_1^2}} \exp\left(-\frac{1}{2\sigma_1^2}(y_i - \mu_1)^2\right) + \frac{w_2}{\sqrt{2\pi\sigma_2^2}} \exp\left(-\frac{1}{2\sigma_2^2}(y_i - \mu_2)^2\right)$$

Can you look at this equation and see what θ achieves maximum likelihood?

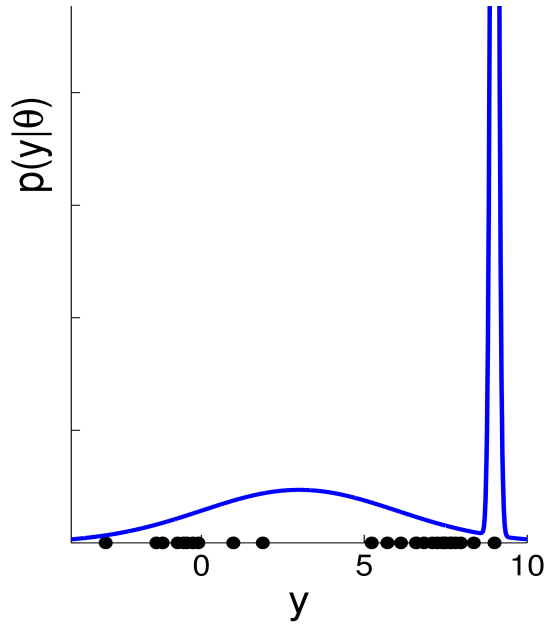
Regularization = MAP $\neq$ Bayesian Inference

Regularization or MAP

- Find

$$\text{argmax}_\theta \log p(\theta|\mathbf{y}) \stackrel{c}{=} \overbrace{\log p(\mathbf{y}|\theta)}^{\text{model fit}} + \overbrace{\log p(\theta)}^{\text{complexity penalty}}$$

- Choose $p(\theta)$ such that $p(\theta) \to 0$ faster than $p(\mathbf{y}|\theta) \to \infty$ as σ_1 or $\sigma_2 \to 0$.



Bayesian Inference

- Predictive Distribution: $p(y_*|\mathbf{y}) = \int p(y_*|\theta)p(\theta|\mathbf{y})d\theta$.
- Parameter Posterior: $p(\theta|\mathbf{y}) \propto p(\mathbf{y}|\theta)p(\theta)$.

Approximate Inference

Ultimately we wish to compute a Bayesian model average:

$$p(y|x_*, \mathcal{D}) = \int p(y|x_*, w)p(w|\mathcal{D})dw\,. \tag{32}$$

For most models, including Bayesian neural networks, this integral is *not analytic*. It is common to use a *Simple Monte Carlo* approximation:

$$p(y|x_*, \mathcal{D}) \approx \frac{1}{J}\sum_j p(y|x_*, w_j)\,, \quad w_j \sim q(w|\mathcal{D})\,. \tag{33}$$

w_j are samples from an approximate posterior $q(w|\mathcal{D})$ typically found by:

1. **Deterministic Methods:** Approximate $p(w|\mathcal{D})$ with convenient $q(w|\mathcal{D}, \theta)$, often Gaussian. θ (e.g. mean of q) chosen to make q close to p. Variational methods find $\text{argmin}_\theta \mathcal{KL}(q||p)$. Classical training: $q(w|\mathcal{D}) = \delta(w = w_{\text{MAP}})$.
   E.g.: Laplace, Expectation Propagation, Variational, Standard Training.
2. **MCMC:** Form a Markov chain of approximate (but asymptotically exact) samples from $p(w|\mathcal{D})$.
   E.g.: Metropolis-Hastings, Hamiltonian Monte Carlo, SGLD, SGHMC.

- Later we will argue we may want to avoid the simple MC perspective.