Back to Maximum Likelihood

- Given a generative model

$$f(x, y = k) = \pi_k f_k(x)$$

- Using a generative modelling approach, we assume a parametric form for $f_k(x) = f(x; \phi_k)$ and compute the MLE $\widehat{\theta}$ of $\theta = (\pi_k, \phi_k)_{k=1}^K$ based on the training data $\{x_i, y_i\}_{i=1}^n$.
- We then use a plug-in approach to perform classification

$$p(Y = k|X = x, \widehat{\theta}) = \frac{\widehat{\pi}_k f(x; \widehat{\phi}_k)}{\sum_{j=1}^K \widehat{\pi}_j f(x; \widehat{\phi}_j)}$$

- Even for simple models, this can prove difficult; e.g. for LDA, $f(x; \phi_k) = \mathcal{N}(x; \mu_k, \Sigma)$, and the MLE estimate of Σ is not full rank for $p > n$.
- One answer: simplify even further, e.g. using axis-aligned covariances, but this is usually too crude.
- Another answer: regularization.

Naïve Bayes

- Return to the spam classification example with two-class naïve Bayes

$$f(x_i; \phi_k) = \prod_{j=1}^p \phi_{kj}^{x_{ij}} (1 - \phi_{kj})^{1-x_{ij}}.$$

The MLE estimates are given by

$$\widehat{\phi}_{kj} = \frac{\sum_{i=1}^n \mathbb{1}(x_{ij} = 1, y_i = k)}{n_k}, \quad \widehat{\pi}_k = \frac{n_k}{n}$$

where $n_k = \sum_{i=1}^n \mathbb{I}(y_i = k)$.
- If a word j does not appear in class k by chance, but it does appear in a document x_*, then $p(x_*|y_* = k) = 0$ and so posterior $p(y_* = k|x_*) = 0$.
- Worse things can happen: e.g., probability of document under all classes can be 0, so posterior is ill-defined.

The Bayesian Learning Framework

- **Bayes Theorem**: Given two random variables X and Θ,

$$p(\Theta|X) = \frac{p(X|\Theta)p(\Theta)}{p(X)}$$

  - **Likelihood**: $p(X|\Theta)$
  - **Prior**: $p(\Theta)$
  - **Posterior**: $p(\Theta|X)$
  - **Marginal likelihood**: $p(X) = \int p(X|\Theta)p(\Theta)d\Theta$
- Treat parameters as random variables, and process of learning is just computation of posterior $p(\Theta|X)$.
- Summarizing the posterior:
  - **Posterior mode**: $\widehat{\theta}^{\text{MAP}} = \text{argmax}_\theta\, p(\theta|X)$. **Maximum a posteriori**.
  - **Posterior mean**: $\widehat{\theta}^{\text{mean}} = \mathbb{E}[\Theta|X]$.
  - **Posterior variance**: $\text{Var}[\Theta|X]$.
- How to make decisions and predictions? Decision theory.
- How to compute posterior?

Simple Example: Coin Tosses

- A very simple example: We have a coin with probability ϕ of coming up heads. Model coin tosses as iid Bernoullis, $1 =$head, $0 =$tail.
- Learn about ϕ given dataset $D = (x_i)_{i=1}^n$ of tosses.

$$f(D|\phi) = \phi^{n_1}(1 - \phi)^{n_0}$$

with $n_j = \sum_{i=1}^n \mathbb{1}(x_i = j)$.
- Maximum likelihood

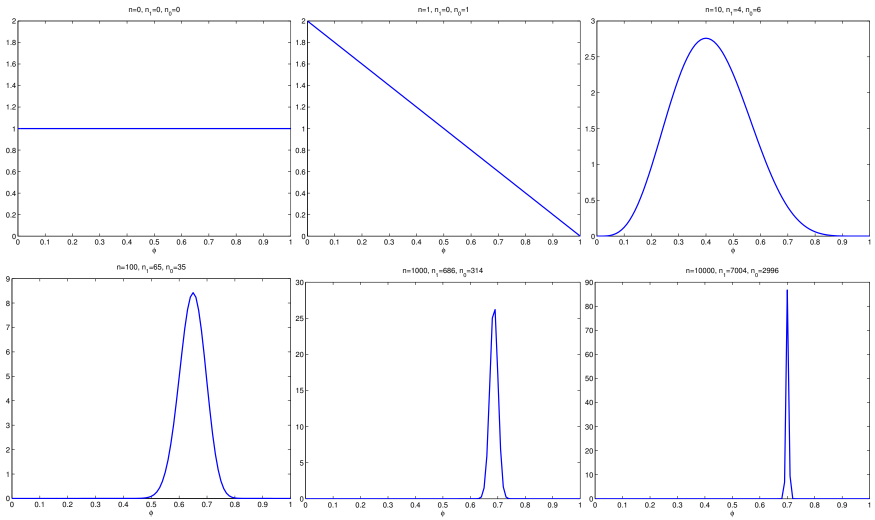
$$\hat{\phi}^{\text{ML}} = \frac{n_1}{n}$$

- Bayesian approach: treat unknown parameter as a random variable Φ. Simple prior: $\Phi \sim U[0, 1]$. Posterior distribution:

$$p(\phi|D) = \frac{1}{Z}\phi^{n_1}(1 - \phi)^{n_0}, \qquad Z = \int_0^1 \phi^{n_1}(1 - \phi)^{n_0} d\phi = \frac{(n + 1)!}{n_1! n_0!}$$

Posterior is a $\text{Beta}(n_1 + 1, n_0 + 1)$ distribution.

Simple Example: Coin Tosses



Posterior becomes peaked at true value $\phi^* = .7$ as dataset grows.

Simple Example: Coin Tosses

- Posterior distribution captures all learnt information.
  - Posterior mode:
    $$\widehat{\phi}^{\text{MAP}} = \frac{n_1}{n}$$
  - Posterior mean:
    $$\widehat{\phi}^{\text{mean}} = \frac{n_1 + 1}{n + 2}$$
  - Posterior variance:
    $$\frac{1}{n+3}\widehat{\phi}^{\text{mean}}(1 - \widehat{\phi}^{\text{mean}})$$
- Asymptotically, for large n, variance decreases as $1/n$ and is given by the inverse of Fisher's information.
- Posterior distribution converges to true parameter ϕ^* as $n \to \infty$.

Simple Example: Coin Tosses

- What about test data?
- The **posterior predictive distribution** is the conditional distribution of x_{n+1} given $(x_i)_{i=1}^n$:

$$\begin{aligned} p(x_{n+1}|(x_i)_{i=1}^n) &= \int_0^1 p(x_{n+1}|\phi, (x_i)_{i=1}^n)p(\phi|(x_i)_{i=1}^n)d\phi \\ &= \int_0^1 p(x_{n+1}|\phi)p(\phi|(x_i)_{i=1}^n)d\phi \\ &= (\widehat{\phi}^{\text{mean}})^{x_{n+1}}(1 - \widehat{\phi}^{\text{mean}})^{1-x_{n+1}} \end{aligned}$$

- We predict on new data by **averaging** the predictive distribution over the posterior. Accounts for uncertainty about ϕ.

Simple Example: Coin Tosses

- Posterior distribution is a known analytic form. In fact posterior distribution is in the same beta family as the prior.
- An example of a **conjugate prior**.
- A beta distribution $\text{Beta}(a, b)$ with parameters $a, b > 0$ is an exponential family distribution with density

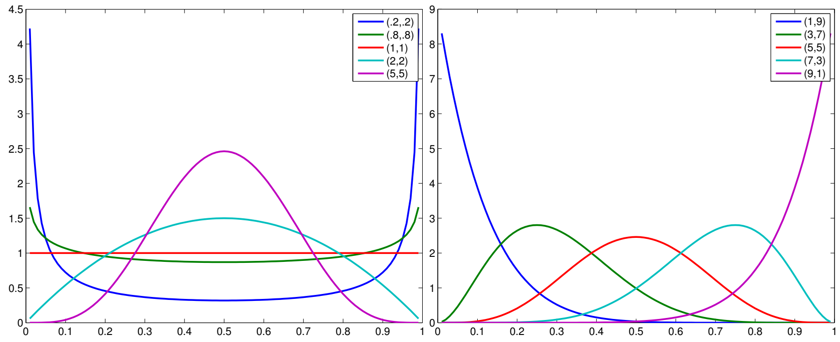
  $$p(\phi|a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\phi^{a-1}(1-\phi)^{b-1}$$

  where $\Gamma(t) = \int_0^\infty u^{t-1}e^{-u}du$ is the gamma function.
- If the prior is $\phi \sim \text{Beta}(a, b)$, then the posterior distribution is

  $$p(\phi|D, a, b) =\propto \phi^{a+n_1-1}(1-\phi)^{b+n_0-1}$$

  so is $\text{Beta}(a + n_1, b + n_0)$.
- Hyperparameters a and b are **pseudo-counts**, an imaginary initial sample that reflects our prior beliefs about ϕ.

Beta Distributions



Bayesian Inference for Multinomials

- Suppose $x_i \in \{1, \ldots, K\}$ instead, and we model $(x_i)_{i=1}^n$ as iid multinomials:

$$p(D|\pi) = \prod_{i=1}^{n} \pi_{x_i} = \prod_{k=1}^{K} \pi_k^{n_k}$$

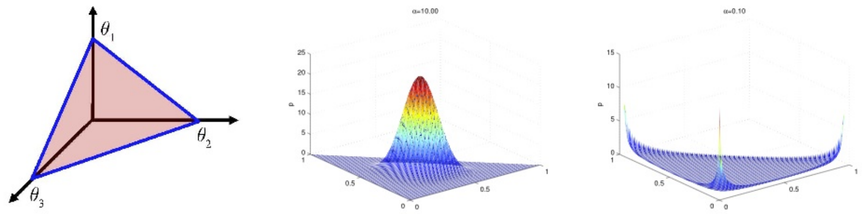
  with $n_k = \sum_{i=1}^n \mathbb{1}(x_i = k)$ and $\pi_k > 0$, $\sum_{k=1}^K \pi_k = 1$.
- The conjugate prior is the Dirichlet distribution. $\mathrm{Dir}(\alpha_1, \ldots, \alpha_K)$ has parameters $\alpha_k > 0$, and density

$$p(\pi) = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$

  on the probability simplex $\{\pi : \pi_k > 0, \sum_{k=1}^K \pi_k = 1\}$.
- The posterior is also Dirichlet, with parameters $(\alpha_k + n_k)_{k=1}^K$.
- Posterior mean is

$$\widehat{\pi}_k^{\text{mean}} = \frac{\alpha_k + n_k}{\sum_{j=1}^K \alpha_j + n_j}$$

Dirichlet Distributions



(A) Support of the Dirichlet density for $K = 3$.
(B) Dirichlet density for $\alpha_k = 10$.
(C) Dirichlet density for $\alpha_k = 0.1$.

Text Classification with (Less) Naïve Bayes

- Under the Naïve Bayes model, the joint distribution of labels $y_i \in \{1, \ldots, K\}$ and data vectors $x_i \in \{0, 1\}^p$ is

$$\prod_{i=1}^{n} p(x_i, y_i) = \prod_{i=1}^{n} \prod_{k=1}^{K} \left(\pi_k \prod_{j=1}^{p} \phi_{kj}^{x_{ij}} (1 - \phi_{kj})^{1 - x_{ij}} \right)^{\mathbb{1}(y_i = k)}$$
$$= \prod_{k=1}^{K} \pi_k^{n_k} \prod_{j=1}^{p} \phi_{kj}^{n_{kj}} (1 - \phi_{kj})^{n_k - n_{kj}}$$

  where $n_k = \sum_{i=1}^n \mathbb{1}(y_i = k)$, $n_{kj} = \sum_{i=1}^n \mathbb{1}(y_i = k, x_{ij} = 1)$.
- For conjugate prior, we can use $\mathrm{Dir}((\alpha_k)_{k=1}^K)$ for π, and $\mathrm{Beta}(a, b)$ for ϕ_{kj} independently.
- Because the likelihood factorizes, the posterior distribution over π and (ϕ_{kj}) also factorizes, and posterior for π is $\mathrm{Dir}((\alpha_k + n_k)_{k=1}^K)$, and for ϕ_{kj} is $\mathrm{Beta}(a + n_{kj}, b + n_k - n_{kj})$.

Text Classification with (Less) Naïve Bayes

- For prediction give $D = (x_i, y_i)_{i=1}^n$ we can calculate

$$p(x_0, y_0 = k|D) = p(y_0 = k|D)p(x_0|y_0 = k, D)$$

with

$$p(y_0 = k|D) = \frac{\alpha_k + n_k}{n + \sum_{l=1}^K \alpha_l}$$
$$p(x_{0j} = 1|y_0 = k, D) = \frac{a + n_{kj}}{a + b + n_k}$$

- Predicted class is

$$p(y_0 = k|x_0|D) = \frac{p(y_0 = k|D)p(x_0|y_0 = k, D)}{p(x_0|D)}$$

- Compared to ML plug-in estimator, pseudocounts help to regularize probabilities away from extreme values.

Bayesian Learning and Regularization

- Consider a Bayesian approach to logistic regression: introduce a multivariate normal prior for b, and uniform (improper) prior for a. The prior density is:

$$p(a, b) = (2\pi\sigma^2)^{-\frac{p}{2}} e^{-\frac{1}{2\sigma^2}\|b\|_2^2}$$

- The posterior is

$$p(a, b|D) \propto \exp\left(-\frac{1}{2\sigma^2}\|b\|_2^2 - \sum_{i=1}^n \log(1 + \exp(-y_i(a + b^\top x_i)))\right)$$

- The posterior mode is the parameters maximizing the above, equivalent to minimizing the L_2-regularized empirical risk.
- Regularized empirical risk minimization is (often) equivalent to having a prior and finding the maximum a posteriori (MAP) parameters.
  - L_2 regularization - multivariate normal prior.
  - L_1 regularization - multivariate Laplace prior.
- From a Bayesian perspective, the MAP parameters are just one way to summarize the posterior distribution.

Bayesian Learning – Discussion

- Clear separation between models, which frame learning problems and encapsulates prior information, and algorithms, which computes posteriors and predictions.
- Bayesian computations — Most posteriors are intractable, and algorithms needed to efficiently approximate posterior:
  - Monte Carlo methods (Markov chain and sequential varieties).
  - Variational methods (variational Bayes, belief propagation etc).
- No optimization — no overfitting (!) but there can still be model misfit.
- Tuning parameters Ψ can be optimized (without need for cross-validation).

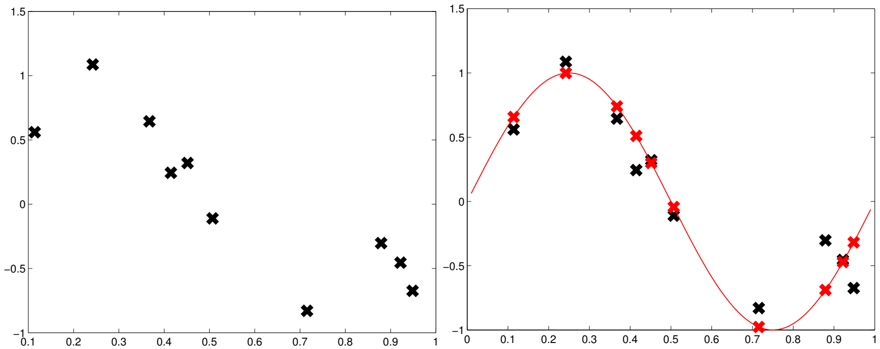
$$p(X|\Psi) = \int p(X|\theta)p(\theta|\Psi)d\theta$$
$$p(\Psi|X) = \frac{p(X|\Psi)p(\Psi)}{p(X)}$$

  - Be Bayesian about Ψ — compute posterior.
  - Type II maximum likelihood — find Ψ maximizing $p(X|\Psi)$.

Bayesian Learning – Further Readings

- Zoubin Ghahramani. Bayesian Learning. Graphical models. Videolectures.
- Gelman et al. Bayesian Data Analysis.
- Kevin Murphy. Machine Learning: a Probabilistic Perspective.

Gaussian Processes



- Suppose we are given a dataset consisting of n inputs $\mathbf{x} = (x_i)_{i=1}^n$ and n outputs $\mathbf{y} = (y_i)_{i=1}^n$.
- Regression: learn the underlying function $f(x)$.

Gaussian Processes

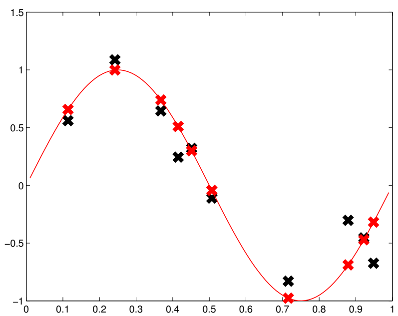
- We can model response as noisy version of an underlying function $f(x)$:

$$y_i | f(x_i) \sim \mathcal{N}(f(x_i), \sigma^2)$$

- Typical approach: parametrize $f(x; \beta)$, and learn β, e.g.,

$$f(x) = \sum_{j=1}^{d} \beta_d \phi_j(x)$$

- More direct approach: since $f(x)$ is unknown, we take a Bayesian approach, introduce a prior over functions, and compute a posterior over functions.



- Instead of trying to work with the whole function, just work with the function values at the inputs

$$\mathbf{f} = (f(x_1), \ldots, f(x_n))^\top$$

Gaussian Processes

- The prior $p(\mathbf{f})$ encodes our prior knowledge about the function.
- What properties of the function can we incorporate?
  - Multivariate normal assumption:

$$\mathbf{f} \sim \mathcal{N}(0, G)$$

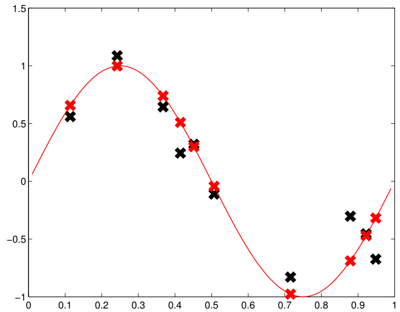
  - Use a kernel function κ to define G:

$$G_{ij} = \kappa(x_i, x_j)$$

  - Expect regression functions to be smooth: If x and x' are close by, then $f(x)$ and $f(x')$ have similar values, i.e. strongly correlated.

$$\begin{pmatrix} f(x) \\ f(x') \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \kappa(x,x) & \kappa(x,x') \\ \kappa(x',x) & \kappa(x',x') \end{pmatrix} \right)$$

  In particular, want $\kappa(x, x') \approx \kappa(x, x) = \kappa(x', x')$.



- Model:

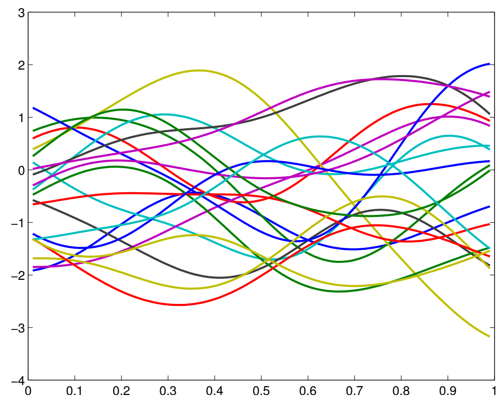
$$\mathbf{f} \sim \mathcal{N}(0, G)$$
$$y_i | f_i \sim \mathcal{N}(f_i, \sigma^2)$$

Gaussian Processes

- What does a multivariate normal prior mean?
- Imagine $\mathbf{x}$ forms a very dense grid of data space. Simulate prior draws

$$\mathbf{f} \sim \mathcal{N}(0, G)$$

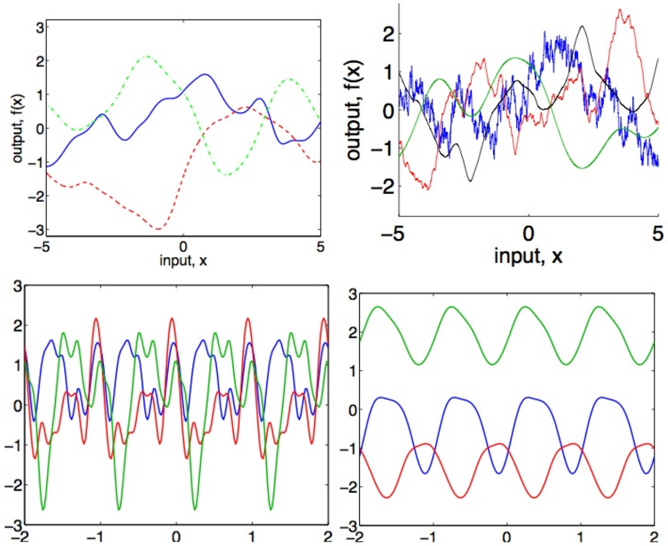
  Plot f_i vs x_i for $i = 1, \ldots, n$.
- The prior over functions is called a **Gaussian process** (GP).



http://www.gaussianprocess.org/

Gaussian Processes

- Different kernels lead to different function characteristics.



Carl Rasmussen. Tutorial on Gaussian Processes at NIPS 2006.

Gaussian Processes

$$\mathbf{f}|\mathbf{x} \sim \mathcal{N}(0, G)$$
$$\mathbf{y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, \sigma^2 I)$$

- Posterior distribution:

$$\mathbf{f}|\mathbf{y} \sim \mathcal{N}(G(G+\sigma^2 I)^{-1}\mathbf{y}, G - G(G+\sigma^2 I)G)$$

- Posterior predictive distribution: Suppose $\mathbf{x}'$ is a test set. We can extend our model to include the function values $\mathbf{f}'$ at the test set:

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}' \end{pmatrix} |\mathbf{x}, \mathbf{x}' \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K_{\mathbf{xx}} & K_{\mathbf{xx}'} \\ K_{\mathbf{x}'\mathbf{x}} & K_{\mathbf{x}'\mathbf{x}'} \end{pmatrix} \right)$$
$$\mathbf{y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, \sigma^2 I)$$

where $K_{\mathbf{zz}'}$ is matrix with ijth entry $\kappa(z_i, z_j')$. $K_{\mathbf{xx}} = G$.

- Some manipulation of multivariate normals gives:

$$\mathbf{f}'|\mathbf{y} \sim \mathcal{N}\left(K_{\mathbf{x}'\mathbf{x}}(K_{\mathbf{xx}}+\sigma^2 I)^{-1}\mathbf{y}, K_{\mathbf{x}'\mathbf{x}'} - K_{\mathbf{x}'\mathbf{x}}(K_{\mathbf{xx}}+\sigma^2 I)^{-1}K_{\mathbf{xx}'}\right)$$

Gaussian Processes