### Laplace Approximation (Contd) and Generalized Linear Models

CS772A: Probabilistic Machine Learning Piyush Rai

# Logistic Regression

There are other ways too that can convert the score into a probability, such as a CDF:  $p(y = 1 | x, w) = \mu = \Phi(w^T x)$  where  $\Phi$  is the CDF of  $\mathcal{N}(0,1)$ . This model is known as "Probit Regression".



- A discriminative model for binary classification  $(y \in \{0,1\})$
- A linear model with parameters  $w \in \mathbb{R}^D$  computes a score  $w^\top x$  for input x
- A sigmoid function maps this real-valued score into probability of label being f 1

$$p(y = 1 | \boldsymbol{x}, \boldsymbol{w}) = \mu = \boldsymbol{\sigma}(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x})$$



 $\blacksquare$  Thus conditional distribution of label  $y \in \{0,1\}$  given x is the following Bernoulli

Likelihood  

$$p(y|\mathbf{x}, \mathbf{w}) = \text{Bernoulli}[y|\mu] = \mu^{y}(1-\mu)^{1-y} = \left[\frac{\exp(\mathbf{w}^{\mathsf{T}}\mathbf{x})}{1+\exp(\mathbf{w}^{\mathsf{T}}\mathbf{x})}\right]^{y} \left[\frac{1}{1+\exp(\mathbf{w}^{\mathsf{T}}\mathbf{x})}\right]^{1-y}$$

• Can use a Gaussian prior on  $w: p(w|\lambda) = \mathcal{N}(w|\mathbf{0}, \lambda^{-1}I)^{-1}$  Can also use a sparsity-inducing prior, such as spike-and-slab or a scale-mixture of Gaussians

- Point estimation (MLE/MAP) for LR gives global optima (NLL is convex in  $\boldsymbol{w}$ )
- We will mainly focus on fully Bayesian inference (computing the posterior)cs772A: PML



### LR Posterior: An Illustration

Assuming the Gaussian approximation, some samples from the posterior of LR



Not all separators from from the posterior are equally good; their "goodness" will depends on their posterior probabilities p(w|X, y)

When making predictions, we can still use all of them but weighted by their importance based on their posterior probabilities

That's exactly what we do when computing the predictive distribution

- Each sample drawn from p(w|X, y) will give a weight vector
- Each such  $\boldsymbol{w}$  corresponds to one of the separators in the above figure



### LR: Posterior Predictive Distribution

The posterior predictive distribution can be computed as

$$p(y_* = 1 | x_*, X, y) = \int p(y_* = 1 | w, x_*) p(w | X, y) dw$$
Integral not tractable and  
must be approximated sigmoid Gaussian (if using Laplace approx.)

- Monte-Carlo approximation of this integral is one possible way
  - Draw M samples  $w_1, w_2, \dots, w_M$ , from the approx. of posterior
  - Approximate the PPD as follows

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{X}, \mathbf{y}) \approx \frac{1}{M} \sum_{m=1}^{M} p(y_* = 1 | \mathbf{w}_m, \mathbf{x}_*) = \frac{1}{M} \sum_{m=1}^{M} \sigma(\mathbf{w}_m^{\mathsf{T}} \mathbf{x}_n)$$

In contrast, when using MLE/MAP solution  $\widehat{w}_{opt}$ , the plug-in pred. distribution

$$p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}) = \int p(y_* = 1 | \boldsymbol{w}, \boldsymbol{x}_*) p(\boldsymbol{w} | \boldsymbol{X}, \boldsymbol{y}) d\boldsymbol{w}$$
  
 
$$\approx p(y_* = 1 | \widehat{\boldsymbol{w}}_{opt}, \boldsymbol{x}_*) = \sigma(\widehat{\boldsymbol{w}}_{opt}^{\mathsf{T}} \boldsymbol{x}_n)$$

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# LR: Plug-in Prediction vs Bayesian Averaging

- Plug-in prediction uses a single w (point est) to make prediction
- $\blacksquare$  PPD does an averaging using all possible w 's from the posterior



### Multiclass Logistic (a.k.a. Softmax) Regression

- Also called multinoulli/multinomial regression: Basically, LR for K > 2 classes
- $\blacksquare$  In this case,  $y_n \in \{1,2,\ldots,K\}$  and label probabilities are defined as

Softmax function  

$$p(y_n = k | \mathbf{x}_n, \mathbf{W}) = \frac{\exp(\mathbf{w}_k^{\mathsf{T}} \mathbf{x}_n)}{\sum_{\ell=1}^{K} \exp(\mathbf{w}_\ell^{\mathsf{T}} \mathbf{x}_n)} = \mu_{nk}$$
Also note that  $\sum_{\ell=1}^{K} \mu_{n\ell} = 1$ 
for any input  $\mathbf{x}_n$ 

- K weight vecs  $w_1, w_2, \dots, w_K$  (one per class), each D-dim, and  $W = [w_1, w_2, \dots, w_K]$
- Each likelihood  $p(y_n | x_n, W)$  is a multinoulli distribution. Therefore total likelihood

$$p(\mathbf{y}|\mathbf{X}, \mathbf{W}) = \prod_{n=1}^{N} \prod_{\ell=1}^{K} \mu_{n\ell}^{y_{n\ell}} - \underbrace{\text{Notation: } y_{n\ell} = 1 \text{ if true class of}}_{\mathbf{X}_n \text{ is } \ell \text{ and } y_{n\ell'} = 0 \forall \ell' \neq \ell}$$

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• Can do MLE/MAP/fully Bayesian estimation for W similar to LR model

## Laplace Approximation of Posterior Distribution

Consider a posterior distribution that is intractable to compute

$$\frac{p(\mathcal{D}|\theta)p(\theta)}{p(\theta|\mathcal{D})} = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} = \frac{p(\mathcal{D},\theta)}{p(\mathcal{D})}$$

Laplace approximation approximates the above using a Gaussian distribution



Why is the above Gaussian a reasonable approximation to the posterior?





• Assuming  $f(\theta) = \log p(\mathcal{D}, \theta)$  and  $\theta_0 = \theta_{MAP}$ ,  $\nabla f(\theta_{MAP}) = \nabla \log p(\mathcal{D}, \theta_{MAP}) = 0$   $\log p(\mathcal{D}, \theta) \approx \log p(\mathcal{D}, \theta_{MAP}) + \frac{1}{2}(\theta - \theta_{MAP})^{\top} \nabla^2 \log p(\mathcal{D}, \theta_{MAP})(\theta - \theta_{MAP})$ • Thus Laplace approx. is based on a second-order Taylor approx. of the posterior

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## Properties of Laplace Approximation

- Usually straightforward if derivatives (first and second) can be computed easily
- Expensive if parameter  $\theta$  is very high dimensional  $\langle very | arge number of features$ 
  - Reason: We need to invert the Hessian whose size is  $D \times D$  (D is the # of params)



- Applicable only when  $\theta$  is real-valued (won't if, say, it is positive, binary etc)
- Note: Even if we have a <u>non-probabilistic</u> model (loss function + regularization), we can obtain an approx "posterior" for that model using the Laplace approximation
  - Optima of the regularized loss function will be Gaussian's mean
  - Second derivative of the regularized loss function will be the Hessian

\*Mixtures of Laplace Approximations for Improved Post-Hoc Uncertainty in Deep Learning (Eschenhagen et al, 2021)

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E.g., a deep neural network, or even in

# Laplace Approx. for High-Dimensional Problems

- $\blacksquare$  When  $\theta$  is very high dim, one option is to approximate the Hessian itself
- One such approx. of the Hessian is a diagonal approximation



- The diagonal approx. of Hessian may be too crude  $oldsymbol{arepsilon}$ 
  - Ignores covariances among params and treats them as being independent of each other
- A block-diagonal approx. proposed recently (in the context of deep neural nets)
  - Treats params across layers to be independent but correlated within the same layer
  - The approach known as Kronecker-Product Factored (KFAC) Laplace approximation

Assuming a discriminative

### Generalized Linear Models

• (Probabilistic) Linear Regression: when response y is real-valued

$$p(y|\boldsymbol{x}, \boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}^{\top}\boldsymbol{x}, \beta^{-1})$$

• Logistic Regression: when response y is binary (0/1)

$$\sigma(\mathbf{y}|\mathbf{x}, \mathbf{w}) = \text{Bernoulli}(\sigma(\mathbf{w}^{\top}\mathbf{x})) = [\sigma(\mathbf{w}^{\top}\mathbf{x})]^{y}[1 - \sigma(\mathbf{w}^{\top}\mathbf{x})]^{1-y}$$
$$\sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$

Note: Probabilistic Linear Regression and Logistic Regression are also GLMs

- In both, the model depends on the inputs  $\boldsymbol{x}$  via a linear model  $\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}$
- Generalized Linear Models (GLM) allow modeling other types of responses, e.g.,
  - Counts (e.g., predicting the hourly hits on a website)
  - Positive reals (e.g., predicting depth of different pixels in a scene, or stock prices)
  - Fractions between 0 and 1 (e.g., predicting proportion of crude oil convertible to gasoline)
- Note: Can convert responses to real values and apply standard regression, but it is better to model them directly (e.g., for better interpretability of the model)



### Generalized Linear Models: Examples

Consider the overdispersed GLMs

$$p(y|\eta,\sigma^2) = h(y,\sigma^2) \exp\left[\frac{\eta y - A(\eta)}{\sigma^2}\right] = \exp\left[\frac{\eta y - A(\eta)}{\sigma^2} + \log h(y,\sigma^2)\right]$$

Consider a linear regression model with Gaussian likelihood

$$p(y|\mathbf{x}, \mathbf{w}, \sigma^2) \propto \exp\left[-\frac{(y - \mathbf{w}^{\mathsf{T}} \mathbf{x})^2}{2\sigma^2}\right] = \exp\left[-\frac{y^2 + (\mathbf{w}^{\mathsf{T}} \mathbf{x})^2 - 2y\mathbf{w}^{\mathsf{T}} \mathbf{x}}{2\sigma^2}\right] = \exp\left[\frac{y\mathbf{w}^{\mathsf{T}} \mathbf{x} - (\mathbf{w}^{\mathsf{T}} \mathbf{x})^2/2}{\sigma^2} - \frac{y^2}{2\sigma^2}\right]$$

• Comparing the expressions, 
$$\eta = w^{T}x$$
,  $A(\eta) = \frac{\eta^{2}}{2}$ ,  $\log h(y, \sigma^{2}) = -y^{2}/2\sigma^{2}$ 

- Can likewise express other models for exp-family distributions  $p(y|\mathbf{x})$ 
  - Regardless of the form, all will have  $\eta = w^{\mathsf{T}} x$



Note that here we expressed the Gaussian in the overdispersed GLM form unlike how we did it earlier when discussing exp-family

## GLM with Canonical Response Function

For GLM with Canon Resp Func (a.k.a., canonical GLM)

$$p(y|\eta) = h(y) \exp(\eta y - A(\eta)) = h(y) \exp(y \mathbf{w}^{\top} \mathbf{x} - A(\eta))^{2}$$

The simple form of canonical GLM (nat. param just a linear function  $\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}$ ) makes parameter estimation via MLE/MAP easy since gradient and Hessian have simple expressions (though the Hessian may be expensive to compute/invert)

- Consider doing MLE (assuming N i.i.d. responses). The log likelihood  $L(\eta) = \log p(Y|\eta) = \log \prod_{n=1}^{N} h(y_n) \exp(y_n w^\top x_n - A(\eta_n)) = \sum_{n=1}^{N} \log h(y_n) + w^\top \sum_{n=1}^{N} y_n x_n - \sum_{n=1}^{N} A(\eta_n)$
- Convexity of  $A(\eta)$  guarantees a global optima. Gradient of log-lik w.r.t. w

$$\mathbf{g} = \sum_{n=1}^{N} \left( y_n \mathbf{x}_n - A'(\eta_n) \frac{d\eta_n}{d\mathbf{w}} \right) = \sum_{n=1}^{N} \left( y_n \mathbf{x}_n - \mu_n \mathbf{x}_n \right) = \sum_{n=1}^{N} \left( y_n - \mu_n \mathbf{x}_n \right) = \sum_{n=1}^{N} \left( y_n - \mu_n \mathbf{x}_n \right) = \sum_{n=1}^{N} \left( y_n - \mu_n \mathbf{x}_n \right) = \mathbf{x}_n$$
The Hessian can also be shown to be

- Note  $\mu_n = f(\xi_n) = f(\mathbf{w}^\top \mathbf{x}_n)$  and  $f = \psi^{-1}$  ("inverse link") depends on the model
  - Real-valued y (linear regression): f is identity, i.e.,  $\mu_n = w^{\mathsf{T}} x_n$
  - Binary y (logistic regression): f is sigmoid function, i.e.,  $\mu_n = \frac{\exp(w^T x_n)}{1 + \exp(w^T x_n)}$
  - Count-valued y (Poisson regression): f is exp, i.e.,  $\mu_n = \exp(\mathbf{w}^T \mathbf{x}_n)$
  - Non-negative y (gamma regression): f is inverse negative i.e.,  $\mu_n = -1/(w^T x_n)$



## Fully Bayesian Inference for GLMs

- Most GLMs, except linear regression with Gaussian lik. and Gaussian prior, do not have conjugate pairs of likelihood and priors (recall logistic regression)
- Posterior over the weight vector w is intractable
- Approximate inference methods needed, e.g.,
  - Laplace approximation (have already seen): Easily applicable since derivatives (first and second) can be easily computed (note that we need  $w_{MAP}$  and Hessian)
  - MCMC or variational inference (will see later)



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### Various Types of GLMs



Type of response	Type of GLM	Link Function $\Psi$	Response Function f (Inv Link Func if canon. GLM) (Operates on $\xi = w^{T}x$ )	Activation
Real	Gaussian	Identity	Identity	Linear
Binary	Logistic	Log-odds: $\log \frac{\mu}{1-\mu}$	Sigmoid	Sigmoid
Binary	Probit	Inv CDF: $\Phi^{-1}(\mu)$	$\Phi$ (CDF of N(0,1))	Probit
Categorical	Multinoulli	Log-odds: $\log \frac{\mu_k}{1-\mu_k}$	Softmax	Softmax
Count	Poisson	$\log \mu$	exp	
Non-negative real	gamma	Negative of inverse	Negative of inverse	
Binary	Gumbel	Gumbel Inv CDF: log(-log())	Gumbel CDF: exp(-exp(-))	

.. and several others (exponential, inverse Gaussian, Binomial, Tweedie, etc)

