Probabilistic Models for Supervised Learning

Piyush Rai

Introduction to Machine Learning (CS771A)

August 16, 2018

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- TA office hours and office locations posted on Piazza (under resources/staff section)

Recap: Probabilistic Modeling

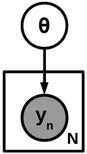

Plate Notation

- A probabilistic model is specified by two key components
  - An observation model $p(\boldsymbol{y}|\theta)$, a.k.a. the likelihood model
  - (Optionally) A prior distribution $p(\theta)$ over the unknown parameters

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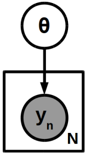

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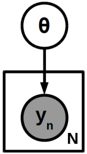

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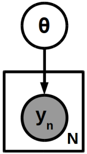

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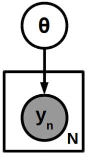

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- We can incorporate our assumptions about the parameters via the prior distribution
- Note: Likelihood and/or prior may depend on additional "hyperparamers" (fixed/unknown)

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  - The integral here may not always be tractable and may need to be approximated

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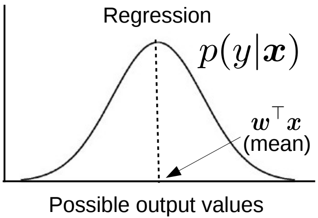
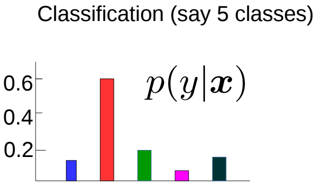
Want models that give us $p(y|x)$

Why Probabilistic Models for Supervised Learning?

- Often, we <u>want</u> the distribution $p(y|\boldsymbol{x})$ over possible outputs y, given an input $\boldsymbol{x}$





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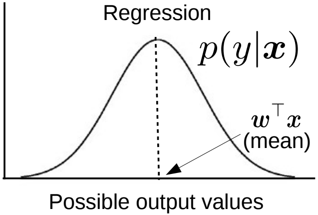

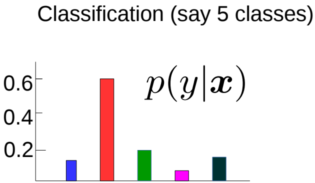

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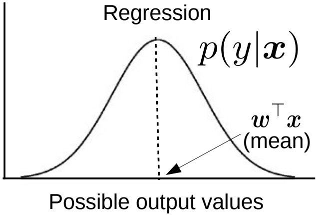

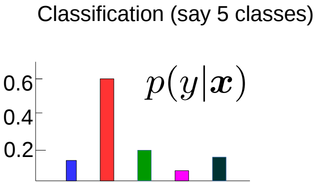

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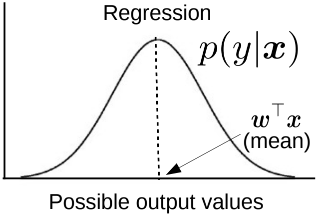

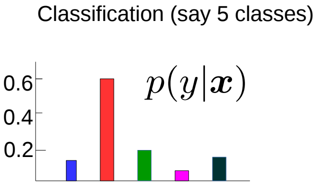

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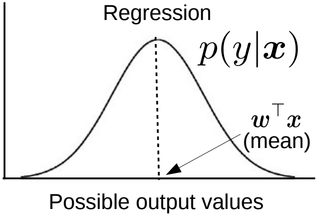

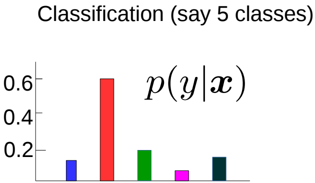

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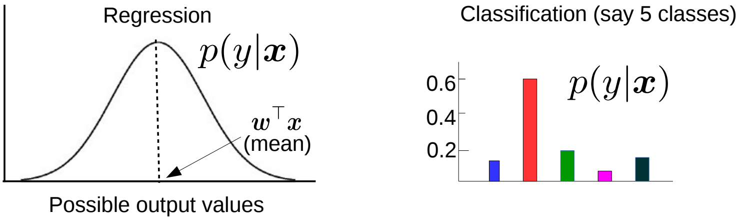

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- Moreover, we can use priors over model parameters, perform fully Bayesian inference, etc.

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(note: $\boldsymbol{w}^\top \boldsymbol{x}$ above only for linear prob. model; can even replace it by a possibly nonlinear $f(\boldsymbol{x})$)

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- **Approach 1:** Don't model $\boldsymbol{x}$, and model $p(y|\boldsymbol{x})$ directly using a prob. distribution, e.g.,

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p(y|\boldsymbol{w},\boldsymbol{x}) &= \mathcal{N}(\boldsymbol{w}^\top\boldsymbol{x},\beta^{-1}) && \text{(prob. linear regression)} \\
p(y|\boldsymbol{w},\boldsymbol{x}) &= \text{Bernoulli}[\sigma(\boldsymbol{w}^\top\boldsymbol{x})] && \text{(prob. linear binary classification)}
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  (note: $\boldsymbol{w}^\top\boldsymbol{x}$ above only for linear prob. model; can even replace it by a possibly nonlinear $f(\boldsymbol{x})$)
- **Approach 2:** Model both $\boldsymbol{x}$ and y via the joint distr. $p(\boldsymbol{x},y)$, and then get the conditional as

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p(y|\boldsymbol{x},\theta) = \frac{p(\boldsymbol{x},y|\theta)}{p(\boldsymbol{x}|\theta)} \quad \text{(note: } \theta \text{ collectively denotes all the parameters)}
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- Approach 1 called Discriminative Modeling; Approach 2 called fully Generative Modeling
  - Discriminative models only model y, not $\boldsymbol{x}$, Generative Models model both y and $\boldsymbol{x}$

Today: Discriminative Models for Probabilistic Regression/Classification

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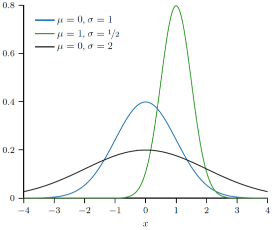
(Also, both are linear models (note the $\boldsymbol{w}^\top \boldsymbol{x}$))

Gaussian Distribution: Brief Review

Univariate Gaussian Distribution

- Distribution over real-valued scalar r.v. x
- Defined by a scalar **mean** μ and a scalar **variance** σ^2
- Distribution defined as

$$\mathcal{N}(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

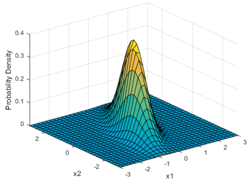


- Mean: $\mathbb{E}[x] = \mu$
- Variance: $\text{var}[x] = \sigma^2$
- Precision (inverse variance) $\beta = 1/\sigma^2$

Multivariate Gaussian Distribution

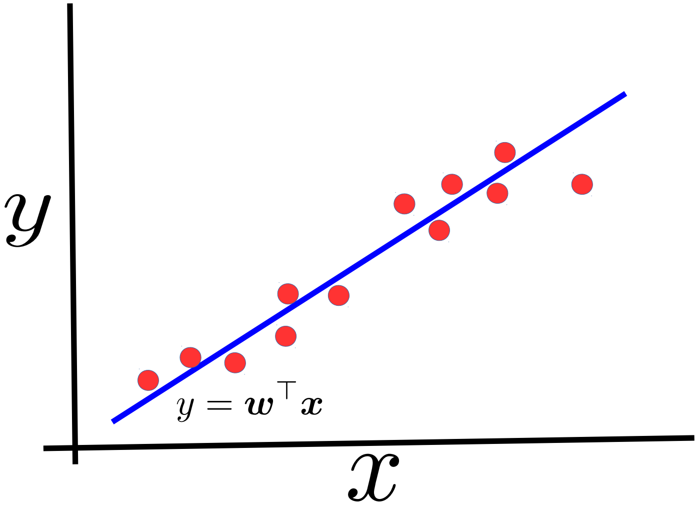
- Distribution over a multivariate r.v. vector $\mathbf{x} \in \mathbb{R}^D$ of real numbers
- Defined by a **mean vector** $\boldsymbol{\mu} \in \mathbb{R}^D$ and a $D \times D$ **covariance matrix** $\boldsymbol{\Sigma}$

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$



- The covariance matrix $\boldsymbol{\Sigma}$ must be symmetric and positive definite
  - All eigenvalues are positive
  - $\boldsymbol{z}^\top \boldsymbol{\Sigma} \boldsymbol{z} > 0$ for any real vector $\boldsymbol{z}$

Linear Regression: A Probabilistic View



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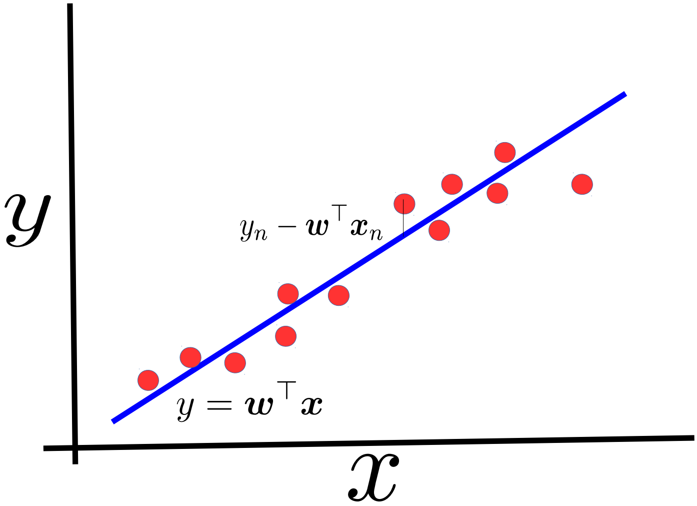

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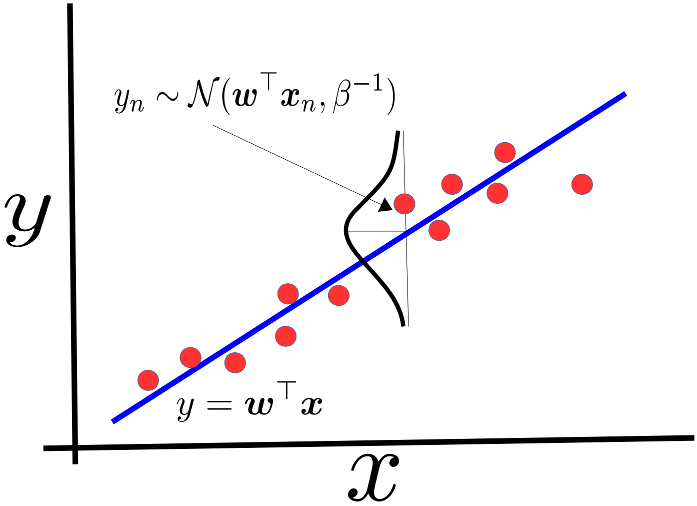

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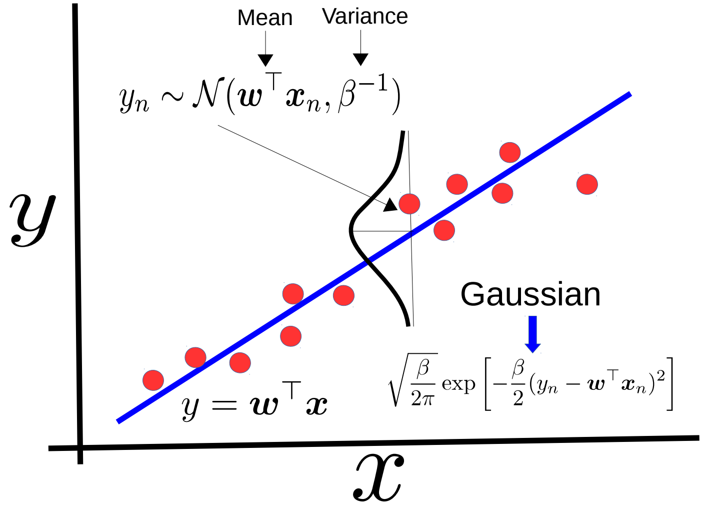

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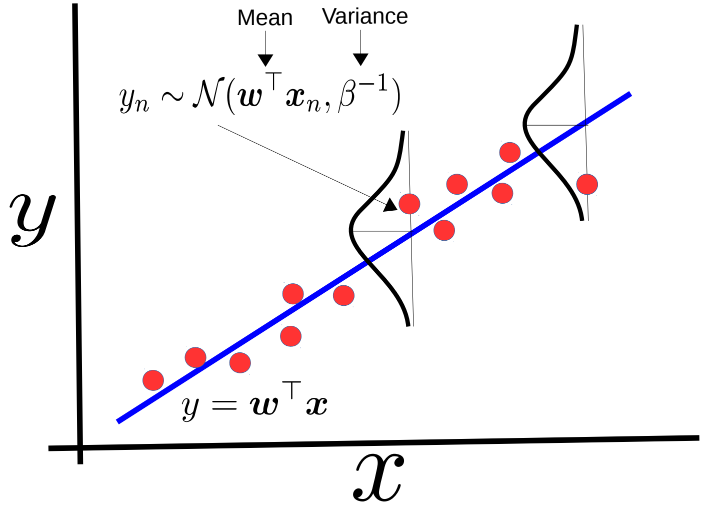

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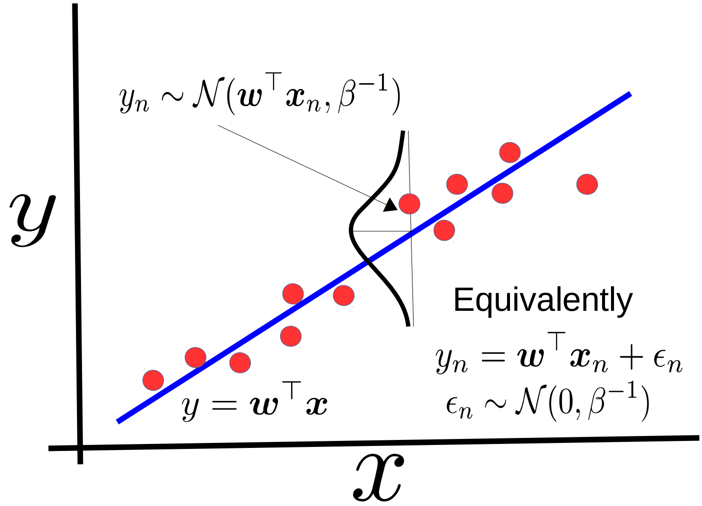
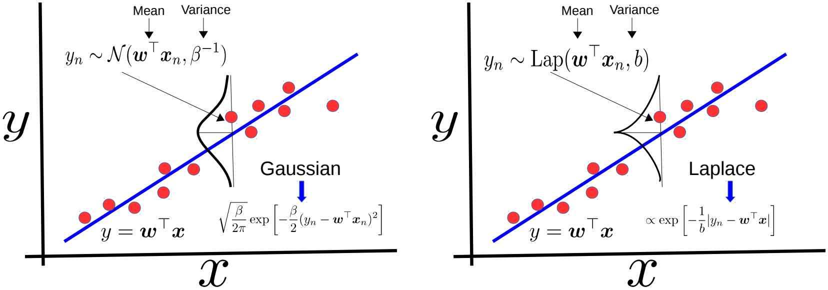


Probabilistic Linear Regression: Some Comments

- Modeling $p(y|\boldsymbol{w}, \boldsymbol{x})$ as a Gaussian $p(y|\boldsymbol{w}, \boldsymbol{x}) = \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}, \beta^{-1})$ is just one possibility
- Can model $p(y|\boldsymbol{w}, \boldsymbol{x})$ using other distributions too, e.g., Laplace (better handles outliers)



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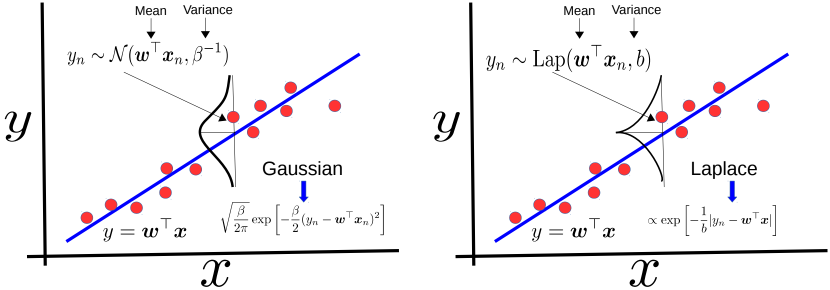

- Even with Gaussian, can assume each output to have a different variance (heteroscedastic noise)

$$p(y|\mathbf{w}, \mathbf{x}_n) = \mathcal{N}(\mathbf{w}^\top \mathbf{x}_n, \beta_n^{-1})$$

MLE for Probabilistic Linear Regression

- Since each likelihood term is a Gaussian, we have

$$p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \beta^{-1}) = \sqrt{\frac{\beta}{2\pi}} \exp\left[-\frac{\beta}{2}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2\right]$$

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- Thus the likelihood (assuming i.i.d. responses) will be

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- Therefor MLE with this model will give the same solution as (unregularized) least squares

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- Let's assume a zero-mean **multivariate Gaussian prior** on weight vector $\boldsymbol{w}$

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- Note that $\frac{\lambda}{\beta}$ is like a regularization hyperparam (as in ridge regression)

Fully Bayesian Inference for Probabilistic Linear Regression

- Can also compute the full posterior distribution over $\boldsymbol{w}$

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$$\begin{aligned} p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X}) &= \mathcal{N}(\boldsymbol{\mu}_N, \boldsymbol{\Sigma}_N) \\ \boldsymbol{\Sigma}_N &= (\beta \mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \\ \boldsymbol{\mu}_N &= (\mathbf{X}^\top \mathbf{X} + \frac{\lambda}{\beta} \mathbf{I}_D)^{-1} \mathbf{X}^\top \boldsymbol{y} \end{aligned}$$

- Note: We are assuming the hyperparameters β and λ to be known
- Note: For brevity, we have omitted the hyperparams from the conditioning in various distributions such as $p(\boldsymbol{w})$, $p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w})$, $p(\boldsymbol{y}|\mathbf{X})$, $p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X})$

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  - Very useful in applications where we want confidence estimates of the predictions made by the model

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  - Other likelihoods/priors can be chosen (result in other loss functions and regularizers)

Discriminative Models for Probabilistic Classification

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(Again, only y will be modeled, $\boldsymbol{x}$ treated as "fixed")

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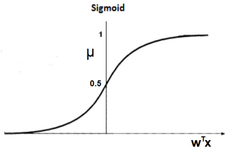

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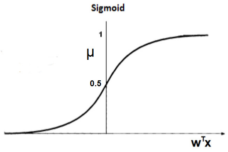

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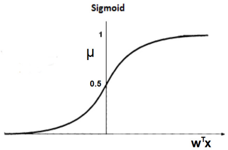

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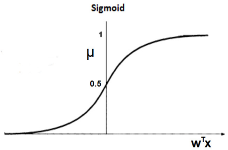

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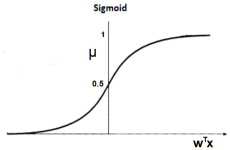

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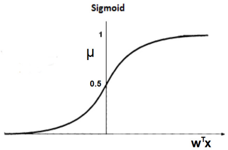

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- **Note:** If we assume $y \in \{-1, +1\}$ instead of $y \in \{0, 1\}$ then $p(y|\boldsymbol{x}, \boldsymbol{w}) = \frac{1}{1+\exp(-y\boldsymbol{w}^\top \boldsymbol{x})}$

Logistic Regression: A Closer Look..

- At the decision boundary where both classes are equiprobable:

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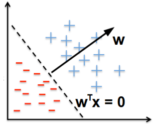
- Therefore $y=1$ if $\boldsymbol{w}^\top \boldsymbol{x} \geq 0$, otherwise $y=0$



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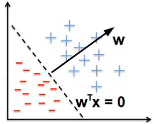

- High positive (negative) score $\boldsymbol{w}^\top \boldsymbol{x}$: High (low) probability of label 1

MLE for Logistic Regression

- Each label $y_n = 1$ with probability $\mu_n = \frac{\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}{1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}$
- Assuming i.i.d. labels, likelihood is product of Bernoullis

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MLE for Logistic Regression

- Each label $y_n = 1$ with probability $\mu_n = \frac{\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}{1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}$
- Assuming i.i.d. labels, likelihood is product of Bernoullis

$$p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \prod_{n=1}^{N} \mu_n^{y_n}(1-\mu_n)^{1-y_n}$$

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  - Exercise: Try computing the gradient of $\text{NLL}(\boldsymbol{w})$ and note the form of the gradient

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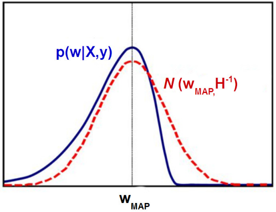
- A crude approximation: **Laplace approximation**: Approximate a posterior by a **Gaussian** with mean $=\boldsymbol{w}_{MAP}$ and covariance $=$ inverse hessian (hessian $=$ second derivative of $\log p(\boldsymbol{w}|\mathbf{X},\boldsymbol{y})$)

$$p(\boldsymbol{w}|\mathbf{X},\boldsymbol{y}) = \mathcal{N}(\boldsymbol{w}_{MAP},\mathbf{H}^{-1})$$



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- Note: Unlike the linear regression case, for logistic regression (and for non-conjugate models in general), posterior averaging can be intractable (and may require approximations)

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    - We can do posterior averagring when computing the predictive distribution
    - Can get variance/confidence estimate in our predictions
- Can model $p(y|\boldsymbol{x})$ direcly (discriminative models) or via $p(\boldsymbol{x}, y)$ (generative models)
- Looked at discriminative models for regression and classification
- Will look at generative models for learning $p(y|\boldsymbol{x})$ next week