Hyperparameter Estimation in Probabilistic Models

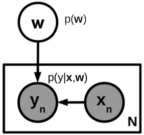
Piyush Rai

Probabilistic Machine Learning (CS772A)

Aug 24, 2017

Hyperparameters

- An example: Recall the linear regression model with Gaussian likelihood and Gaussian prior



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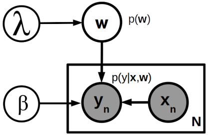

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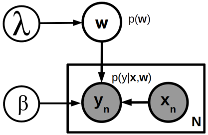

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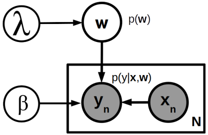

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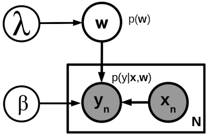

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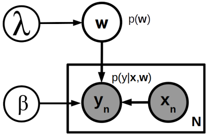

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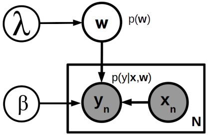

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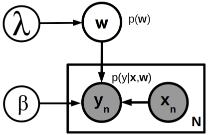

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- Can we learn these hyperparameters from data?

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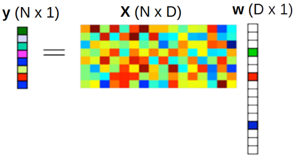

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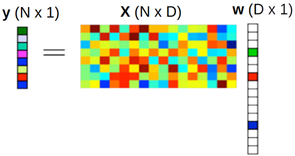

- Tuning is usually impossible to do in unsupervised learning problems (e.g., clustering)

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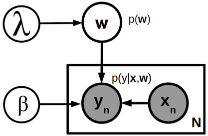

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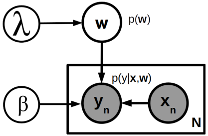

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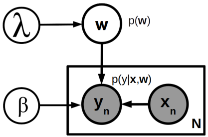

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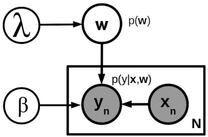

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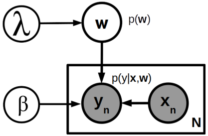

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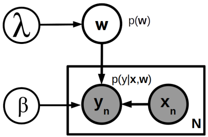

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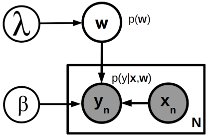

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- Note: If the likelihood and prior are conjugate then marginal likelihood is available in closed form

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- For linear regression case, would ideally like the posterior over all unknowns, i.e., $p(\boldsymbol{w}, \lambda, \beta | \mathbf{X}, \boldsymbol{y})$

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- Moreover, if $p(\beta)$, $p(\lambda)$ are uniform/uninformative priors then

$$\hat{\beta}, \hat{\lambda} = \arg\max_{\beta, \lambda} p(\boldsymbol{y} | \mathbf{X}, \beta, \lambda)$$

What is MLE-II Doing?

- For linear regression case, would ideally like the posterior over all unknowns, i.e., $p(\boldsymbol{w}, \lambda, \beta | \mathbf{X}, \boldsymbol{y})$

$$p(\boldsymbol{w}, \beta, \lambda | \mathbf{X}, \boldsymbol{y}) = p(\boldsymbol{w} | \mathbf{X}, \boldsymbol{y}, \beta, \lambda) p(\beta, \lambda | \mathbf{X}, \boldsymbol{y}) \qquad \text{(from product rule)}$$

- Note that $p(\boldsymbol{w} | \mathbf{X}, \boldsymbol{y}, \beta, \lambda)$ is easy if λ, β are known
- However $p(\beta, \lambda | \mathbf{X}, \boldsymbol{y}) = \frac{p(\boldsymbol{y} | \mathbf{X}, \beta, \alpha) p(\beta) p(\lambda)}{p(\boldsymbol{y} | \mathbf{X})}$ is hard (lack of conjugacy, intractable denominator)
- Let's approximate it by a point function δ at the mode of $p(\beta, \lambda | \mathbf{X}, \boldsymbol{y})$

$$p(\beta, \lambda | \mathbf{X}, \boldsymbol{y}) \approx \delta(\hat{\beta}, \hat{\lambda}) \quad \text{where} \quad \hat{\beta}, \hat{\lambda} = \arg\max_{\beta, \lambda} p(\beta, \lambda | \mathbf{X}, \boldsymbol{y}) = \arg\max_{\beta, \lambda} p(\boldsymbol{y} | \mathbf{X}, \beta, \lambda) p(\lambda) p(\beta)$$

- Moreover, if $p(\beta)$, $p(\lambda)$ are uniform/uninformative priors then

$$\hat{\beta}, \hat{\lambda} = \arg\max_{\beta, \lambda} p(\boldsymbol{y} | \mathbf{X}, \beta, \lambda)$$

- Thus MLE-II is approximating the posterior of hyperparams by their point estimate assuming uniform priors (therefore we don't need to worry about a prior over the hyperparams)

MLE-II for Linear Regression

- For the linear regression case, the marginal likelihood is defined as

$$p(\boldsymbol{y}|\mathbf{X},\beta,\lambda) = \int p(\boldsymbol{y}|\mathbf{X},\boldsymbol{w},\beta)p(\boldsymbol{w}|\lambda)d\boldsymbol{w}$$

where $p(\boldsymbol{y}|\mathbf{X},\boldsymbol{w},\beta) = \mathcal{N}(\boldsymbol{y}|\mathbf{X}\boldsymbol{w},\beta^{-1}\mathbf{I}_N)$ and $p(\boldsymbol{w}|\lambda) = \mathcal{N}(\boldsymbol{w}|0,\lambda^{-1}\mathbf{I}_D)$

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- The above can be computed in closed form, using properties of Gaussians (see below)

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$$p(\boldsymbol{y}|\mathbf{X},\beta,\lambda) = \mathcal{N}(\boldsymbol{y}|\mathbf{0},\beta^{-1}\mathbf{I}+\lambda^{-1}\mathbf{X}\mathbf{X}^\top) = \frac{1}{(2\pi)^{N/2}}|\beta^{-1}\mathbf{I}+\lambda^{-1}\mathbf{X}\mathbf{X}^\top|^{-1/2}\exp(-\frac{1}{2}\boldsymbol{y}^\top(\beta^{-1}\mathbf{I}+\lambda^{-1}\mathbf{X}\mathbf{X}^\top)^{-1}\boldsymbol{y})$$

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    - Usually there is no closed form solution. Solved using iterative/alternating optimization

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We can follow an iterative scheme for estimating $\boldsymbol{w}$, λ, and β

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Note that the update of one parameter depends on the current estimate of other parameters

Using MLE-II Estimates for Making Prediction

- With the MLE-II approximation $p(\beta,\lambda|\mathbf{X},\boldsymbol{y}) \approx \delta(\hat{\beta},\hat{\lambda})$, the posterior over unknowns

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- The posterior predictive distribution can also be approximated as

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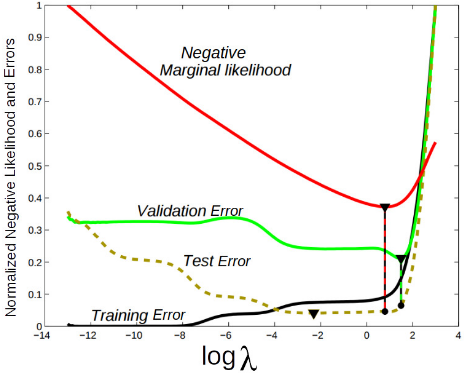
- This is also the same as the usual posterior predictive distribution we have seen earlier, except we are treating the hyperparams $\hat{\beta}, \hat{\lambda}$ fixed at their MLE-II based estimates

Illustration of Hyperparameter Estimation via MLE-II



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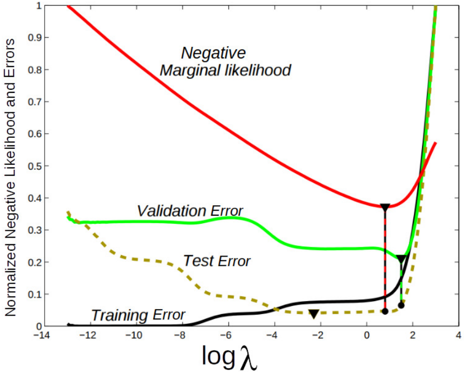
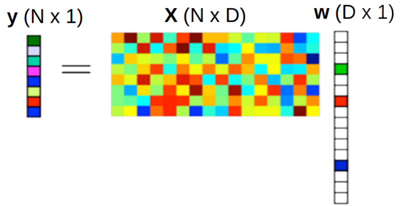


Important: Unlike cross-validation, the marginal lik. based MLE-II approach doesn't need a separate held-out data set (MLE-II uses all the training data for estimating the hyperparameters)

Another Example: Sparse Modeling

- In high-dim regression problems, we want very few elements in $\boldsymbol{w}$ to be nonzero



- We can impose component-wise regularization on $\boldsymbol{w}$ via the following prior

$$p(\boldsymbol{w}) = \prod_{d=1}^{D} \mathcal{N}(w_d|0, \lambda_d^{-1}) = \prod_{d=1}^{D} \left(\frac{\lambda_d}{2\pi}\right)^{1/2} \exp\left(-\frac{\lambda_d}{2} w_d^2\right)$$

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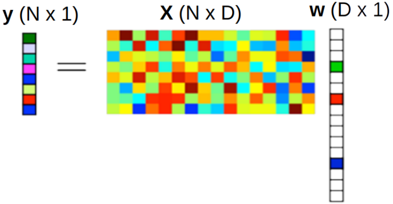

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- With a Gaussian likelihood for $\boldsymbol{y}$, this is called Sparse Bayesian Linear Regression

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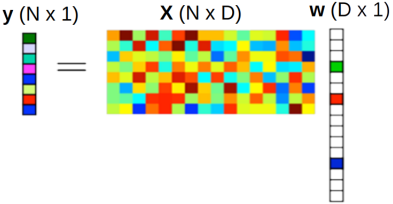

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- With a Gaussian likelihood for $\boldsymbol{y}$, this is called Sparse Bayesian Linear Regression
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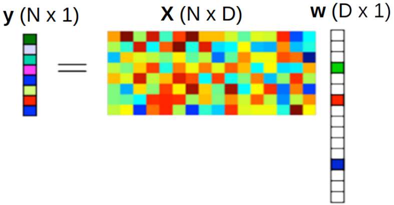
Another Example: Sparse Modeling

- In high-dim regression problems, we want very few elements in $\boldsymbol{w}$ to be nonzero



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- We can again MLE-II to estimate these hyperparameters

MLE-II for Sparse Bayesian Linear Regression

- Posterior over $\boldsymbol{w}$: $p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \boldsymbol{\lambda}, \beta) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Again, easy to compute in closed form.

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- We alternate between estimating $\boldsymbol{w}$, $\boldsymbol{\lambda}$, and β, until we converge

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  - We will discuss this later during the semester