Exponential Family Distributions and Conditional Models

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Topics in Probabilistic Modeling and Inference (CS698X)

Jan 16, 2019

Plan for today

- Exponential family distributions (a very important class of distributions)

$$p(\boldsymbol{x}|\theta) = \frac{1}{Z(\theta)} h(\boldsymbol{x}) \exp[\theta^\top \phi(\boldsymbol{x})] \quad = \quad h(\boldsymbol{x}) \exp[\theta^\top \phi(\boldsymbol{x}) - A(\theta)]$$

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- Conditional models and parameter estimation for them (our example: Prob. Linear Regression)

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

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- $h(\boldsymbol{x})$: A constant (doesn't depend on θ)

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- Now compare the resulting expression with the exponential family form

$$p(\boldsymbol{x}|\theta) = h(\boldsymbol{x})\exp(\theta^\top\phi(\boldsymbol{x}) - A(\theta))$$

.. to identify the natural parameters, sufficient statistics, log-partition function, etc.

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- $A(\theta) = \frac{\mu^2}{2\sigma^2} + \log\sigma = \frac{-\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) - \frac{1}{2}\log(2\pi)$

Other Examples

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  - Beta
  - Gamma
  - Multinoulli/Multinomial
  - Dirichlet
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- Note: Not all distributions belong to the exponential family, e.g.,
  - Uniform distribution ($x \sim \text{Unif}(a, b)$)
  - Student-t distribution
  - Mixture distributions (e.g., mixture of Gaussians)

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- Note: The above result also holds when θ and $\phi(\boldsymbol{x})$ are vector-valued (the "var" will be "covar")

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- Note: The above result also holds when θ and $\phi(\boldsymbol{x})$ are vector-valued (the "var" will be "covar")
- Important: $A(\theta)$ is a **convex function** of θ.

Log-Partition Function

- $A(\theta) = \log Z(\theta) = \log \int h(\boldsymbol{x}) \exp[\theta^\top \phi(\boldsymbol{x})] d\boldsymbol{x}$ is the log-partition function
- $A(\theta)$ is also called the cumulant function
- Derivatives of $A(\theta)$ can be used to generate the cumulants of the sufficient statistics $\phi(\boldsymbol{x})$
- Exercise: Assume θ to be a scalar (thus $\phi(\boldsymbol{x})$ is also scalar). Show that the first and the second derivatives of $A(\theta)$ are

$$\frac{dA}{d\theta} = \mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi(\boldsymbol{x})]$$

$$\frac{d^2 A}{d\theta^2} = \mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi^2(\boldsymbol{x})] - \left[\mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi(\boldsymbol{x})]\right]^2 = \text{var}[\phi(\boldsymbol{x})]$$

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MLE for Exponential Family Distributions

- Suppose we have data $\mathcal{D} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ drawn i.i.d. from an exponential family distribution

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- Only exponential family distributions have finite-sized sufficient statistics
  - No need to store all the data; can simply store and recursively update the sufficient statistics with more and more data
  - Very useful when doing probabilistic/Bayesian inference with large-scale data sets. Also useful in online parameter estimation problems.

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- The likelihood is of the form $p(\mathcal{D}|\theta) = \left[\prod_{i=1}^{N} h(\boldsymbol{x}_i)\right] \exp\left[\theta^\top \phi(\mathcal{D}) - NA(\theta)\right]$
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- This is basically matching the expected moments of the distribution with empirical moments ("empirical" here means what we compute using the observed data)

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Bayesian Inference for Exponential Family Distributions

- We saw that the total likelihood given N i.i.d. observations $\mathcal{D}\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$

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- Note: Prior's log-partition function $A_c(\nu_0, \boldsymbol{\tau}_0)$ updates to posterior's: $A_c(\nu_0 + N, \boldsymbol{\tau}_0 + \phi(\mathcal{D}))$

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- Note that the posterior hyperparam $\bar{\tau}_0'$ is a convex combination of the average suff-stats $\bar{\tau}_0$ of the ν_0 pseudo-observations and the average suff-stats $\bar{\phi}$ of the N actual observations

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  - Gaussian-Gaussian, Gaussian-IG, Gaussian-Gamma, Gaussian-NIG, Gaussian-NG case: Posterior predictive distribution of the next observation
- Nice Property: If the likelihood is an exponential family distribution, prior is conjugate (and thus is the posterior), the posterior predictive always has a closed form expression (shown next)

Posterior Predictive Distribution

- Recall the form of the likelihood $p(\mathcal{D}|\theta)$ for exp. family dist.

$$p(\mathcal{D}|\theta) = \left[\prod_{i=1}^{N} h(\boldsymbol{x}_i)\right] \exp\left[\theta^\top \phi(\mathcal{D}) - NA(\theta)\right]$$

- The conjugate prior was

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- For this choice of the conjugate prior, the posterior was shown to be

$$p(\theta|\mathcal{D}) = h(\theta) \exp\left[\theta^\top (\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta) - A_c(\nu_0 + N, \boldsymbol{\tau}_0 + \phi(\mathcal{D}))\right]$$

Posterior Predictive Distribution

- Recall the form of the likelihood $p(\mathcal{D}|\theta)$ for exp. family dist.

$$p(\mathcal{D}|\theta) = \left[\prod_{i=1}^{N} h(\boldsymbol{x}_i)\right] \exp\left[\theta^\top \phi(\mathcal{D}) - NA(\theta)\right]$$

- The conjugate prior was

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- For the test data $\mathcal{D}'$, the likelihood will be

$$p(\mathcal{D}'|\theta) = \left[\prod_{i=1}^{N'} h(\tilde{\boldsymbol{x}}_i)\right] \exp\left[\theta^\top \phi(\mathcal{D}') - N'A(\theta)\right] \qquad \text{where} \quad \phi(\mathcal{D}') = \sum_{i=1}^{N'} \phi(\tilde{\boldsymbol{x}}_i)$$

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  - Linear regression (with Gaussian likelihood) and logistic regression are GLMs
- We will see several use cases when we discuss approximate inference algoritms (e.g., Gibbs sampling, and especially variational inference)

Estimating Conditional Models, e.g., $p(y|\boldsymbol{x})$

Our Example: Probabilistic/Bayesian Linear Regression

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- Today's focus will be on regression problems (y is real-valued response for the input $\boldsymbol{x}$)

Linear Regression: A Probabilistic Setup

- Given: N training examples $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, features: $\boldsymbol{x}_n \in \mathbb{R}^D$, response $y_n \in \mathbb{R}$

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- Assume a "noisy" linear model with regression weight vector $\boldsymbol{w} = [w_1, w_2, \ldots, w_D] \in \mathbb{R}^D$

$$y_n = \boldsymbol{w}^\top \boldsymbol{x}_n + \epsilon_n$$

where $\epsilon_n \sim \mathcal{N}(0, \beta^{-1})$, β: precision (inverse variance) of Gaussian (assumed known)

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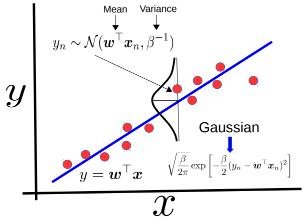


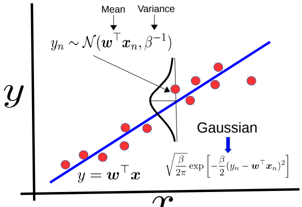
Linear Regression: A Probabilistic Setup

- Given: N training examples $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, features: $\boldsymbol{x}_n \in \mathbb{R}^D$, response $y_n \in \mathbb{R}$
- Assume a "noisy" linear model with regression weight vector $\boldsymbol{w} = [w_1, w_2, \ldots, w_D] \in \mathbb{R}^D$

$$y_n = \boldsymbol{w}^\top \boldsymbol{x}_n + \epsilon_n$$

where $\epsilon_n \sim \mathcal{N}(0, \beta^{-1})$, β: precision (inverse variance) of Gaussian (assumed known)

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



- Note: Some books (e.g., PRML) use $\phi(\boldsymbol{x}_n)$ to denote the features where ϕ is some transformation of the original features $\boldsymbol{x}_n$ (we will only use this notation when talking about nonlinear regression)

The Likelihood Model

- Notation: $\mathbf{X} = [\boldsymbol{x}_1 \dots \boldsymbol{x}_N]^\top$: $N \times D$ feature matrix, $\boldsymbol{y} = [y_1 \dots y_N]^\top$: $N \times 1$ response vector

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- Assuming independent observations, the likelihood model

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

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- Note that NLL = sum of squared errors! Minimizing w.r.t. $\boldsymbol{w}$ will give MLE/least squares solution!

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- Note that NLL = sum of squared errors! Minimizing w.r.t. $\boldsymbol{w}$ will give MLE/least squares solution!
- For brevity, can also write the likelihood $p(\boldsymbol{y}|\boldsymbol{w}, \mathbf{X})$ as an N-dim multivariate Gaussian

$$
p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta) = \mathcal{N}(\boldsymbol{y}|\mathbf{X}\boldsymbol{w}, \beta^{-1}\mathbf{I}_N) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \exp\left[-\frac{\beta}{2}(\boldsymbol{y} - \mathbf{X}\boldsymbol{w})^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{w})\right]
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The Prior

- Assume the entries in $\boldsymbol{w}$ are i.i.d. with zero mean Gaussian priors. Therefore

$$p(\boldsymbol{w}) = \prod_{d=1}^{D} p(w_d) = \prod_{d=1}^{D} \mathcal{N}(w_d|0, \lambda^{-1})$$

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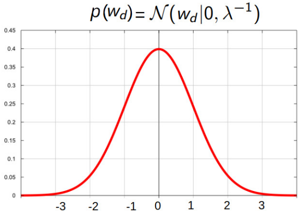

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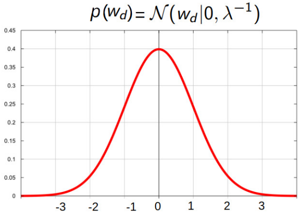

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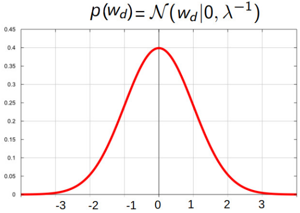
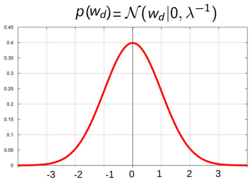


- This prior promotes the entries in $\boldsymbol{w}$ to be small (close to zero)
  - Also, the negative of log-prior is the same as an ℓ_2 regularizer on $\boldsymbol{w}$
- This prior is conjugate to the likelihood (Gaussian) which makes posterior inference easy

The Prior



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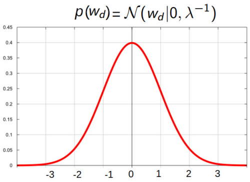

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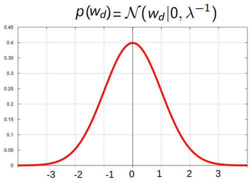

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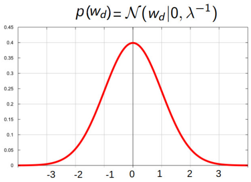

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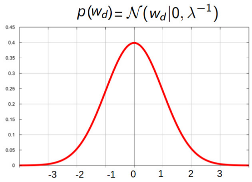

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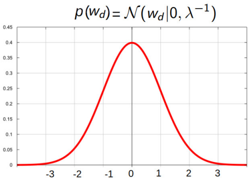

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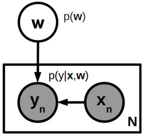
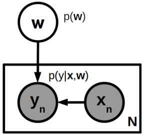
  - Useful in sparse regression/classification models in which very few features are relevant which can be identified by inferring $\{\lambda_d\}_{d=1}^D$. Popularly known as sparse Bayesian learning (more on this later).

Inference Tasks for Bayesian Linear Regression



(Hyperparameters λ,β not shown as they are fixed/known)

Inference Tasks for Bayesian Linear Regression



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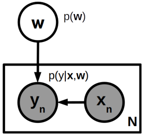

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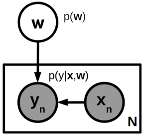

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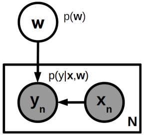

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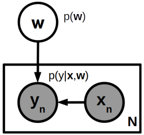

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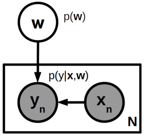
Inference Tasks for Bayesian Linear Regression



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Bayesian Linear Regression: The Posterior

- The posterior over $\boldsymbol{w}$ (for now, assume hyperparams β and λ to be known)

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- Using the "completing the squares" trick (or directly using Gaussian conditioning formula)

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$$\text{where} \quad \boldsymbol{\Sigma}_N = (\beta \sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^\top + \lambda \mathbf{I}_D)^{-1} = (\beta \mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \quad \text{(posterior's covariance matrix)}$$

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- The posterior over $\boldsymbol{w}$ (for now, assume hyperparams β and λ to be known)

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

- Computing $p(\boldsymbol{w}|\mathbf{X},\boldsymbol{y},\beta,\lambda)$

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

- Using the "completing the squares" trick (or directly using Gaussian conditioning formula)

$$\begin{aligned}
p(\boldsymbol{w}|\boldsymbol{y},\mathbf{X},\beta,\lambda) &= \mathcal{N}(\boldsymbol{\mu}_N,\boldsymbol{\Sigma}_N) \\
\text{where} \quad \boldsymbol{\Sigma}_N &= (\beta\sum_{n=1}^{N}\boldsymbol{x}_n\boldsymbol{x}_n^\top + \lambda\mathbf{I}_D)^{-1} = (\beta\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_D)^{-1} \quad \text{(posterior's covariance matrix)} \\
\boldsymbol{\mu}_N &= \boldsymbol{\Sigma}_N\left[\beta\sum_{n=1}^{N}y_n\boldsymbol{x}_n\right] = \boldsymbol{\Sigma}_N\left[\beta\mathbf{X}^\top\boldsymbol{y}\right] = (\mathbf{X}^\top\mathbf{X} + \frac{\lambda}{\beta}\mathbf{I}_D)^{-1}\mathbf{X}^\top\boldsymbol{y} \quad \text{(posterior's mean)}
\end{aligned}$$

The Posterior: A Visualization

- Assume a linear regression problem with ground truth $\boldsymbol{w} = [w_0, w_1]$ with $w_0 = -0.3, w_1 = 0.5$
- Assume data generated by a linear regression model $y = w_0 + w_1 x +$ "noise"
  - Note: It's actually 1-D regression (w_0 is just a bias term), or 2-D reg. with feature $[1, x]$

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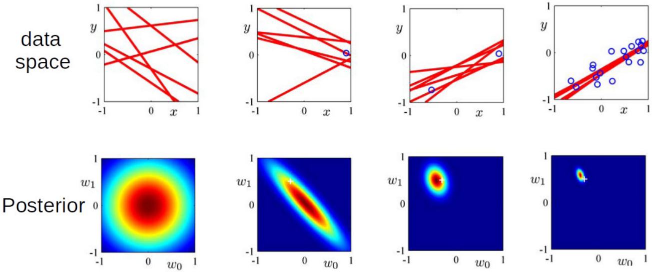

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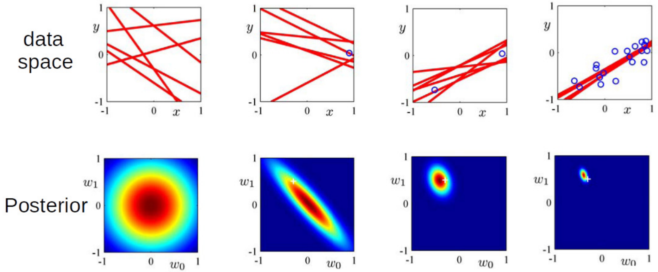

- The "data space" (red lines) shown above denotes various possible linear regression datasets with data of the form $y = w_0 + w_1 x$ generated using $\boldsymbol{w}$ drawn from the current posterior of $\boldsymbol{w}$

Bayesian Linear Regression: Posterior Predictive Distribution

- Given the posterior $p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X}, \beta, \lambda) = \mathcal{N}(\boldsymbol{\mu}_N, \boldsymbol{\Sigma}_N)$, how to make prediction y_* for a new input $\boldsymbol{x}_*$?

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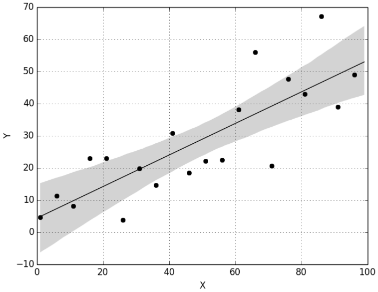
- Important: Unlike MLE/MAP, the variance of y_* also depends on the input $\boldsymbol{x}_*$ (this, as we will see later, will be very useful in sequential decision-making problems such as active learning)

Posterior Predictive Distribution: An Illustration

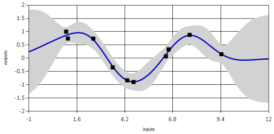
Black dots are training examples



Width of the shaded region at any x denotes the predictive uncertainty at that x (+/- one std-dev)

Regions with more training examples have smaller predictive variance

Nonlinear Regression?



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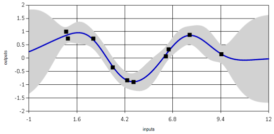

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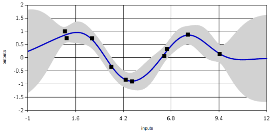

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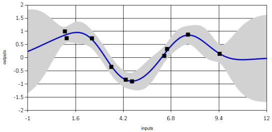

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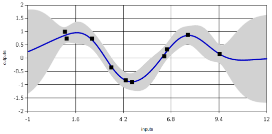

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- More on nonlinear regression when we discuss Gaussian Processes

What about the hyperparameters of the regression model?

- If hyperparameters are to be estimated, we will have a hierarchical/multiparameter model
- Posterior inference in slightly more involved in this case
- Iterative methods required to learn the weight vector and the hyperparameters, e.g.,
  - Marginal likelihood maximization for hyperparameter estimation
  - Expectation maximization (EM)
  - MCMC or variational inference
- We will discuss more when we talk about inference in hierarchical/multiparameter models

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  - Approximate inference methods (e.g., EM, Gibbs sampling, etc) that resemble alternating optimization techniques