STA 414/2104: Machine Learning

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Lecture 10

- Polynomial curve fitting generalization, overfitting
- Decision theory:
 - Minimizing misclassification rate / Minimizing the expected loss



Loss functions for regression

$$\mathbb{E}[L] = \int \int (t - y(\mathbf{x}))^2 p(\mathbf{x}, t) d\mathbf{x} dt.$$

- Bernoulli, Multinomial random variables (mean, variances)
- Multivariate Gaussian distribution (form, mean, covariance)
- Maximum likelihood estimation for these distributions.
- Exponential family / Maximum likelihood estimation / sufficient statistics for exponential family.

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

• Linear basis function models / maximum likelihood and least squares:

$$\begin{aligned} &\ln p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \sum_{i=1}^{N} \ln \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta) \\ &= -\frac{\beta}{2} \sum_{n=1}^{N} \left(t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) \right)^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi). \end{aligned} \mathbf{w}_{\mathrm{ML}} = \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{t} \end{aligned}$$

• Regularized least squares:

$$\frac{1}{2}\sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \qquad \mathbf{w} = \left(\lambda \mathbf{I} + \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t}.$$

- Bayesian interpretation
- Bias-variance decomposition.





Ridge

regression

• Bayesian Inference: likelihood, prior, posterior:

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})P(\mathbf{w})}{P(\mathcal{D})}$$

Marginal likelihood (normalizing constant):

• Marginal likelihood / predictive distribution.

$$P(\mathcal{D}) = \int p(\mathcal{D}|\mathbf{w})P(\mathbf{w})d\mathbf{w}$$

 Bayesian linear regression / parameter estimation / posterior distribution / predictive distribution

Bayesian model comparison / Evidence approximation



- Classification models:
 - Discriminant functions
 - Fisher's linear discriminant

 Probabilistic Generative Models / Gaussian class conditionals / Maximum likelihood estimation:

$$p(\mathbf{x}|\mathcal{C}_{k}) = \frac{1}{(2\pi)^{D/2}|\mathbf{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_{k})^{T}\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_{k})\right).$$

$$p(\mathcal{C}_{k}|\mathbf{x}) = \sigma(\mathbf{w}^{T}\mathbf{x}+w_{0}),$$

$$\mathbf{w} = \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_{1}-\boldsymbol{\mu}_{2}),$$

$$w_{0} = -\frac{1}{2}\boldsymbol{\mu}_{1}^{T}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_{1} + \frac{1}{2}\boldsymbol{\mu}_{2}^{T}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_{2} + \ln\frac{p(\mathcal{C}_{1})}{p(\mathcal{C}_{2})}.$$

• Discriminative Models / Logistic regression / maximum likelihood estimation

• Gaussian processes, definition:

$$\begin{bmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} m(\mathbf{x}_1) \\ \vdots \\ m(\mathbf{x}_N) \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & \cdots & k(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix} \right)$$

- GPs for regression.
- Marginal/predictive distributions. Making predictions using GPs.
- Covariance functions, automatic relevance determination, role of hyperparameters



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

- Mixture Models, k-means, Mixture of Gaussians
- Mixture of Gaussians: Maximum likelihood estimation.
- EM algorithm: definition of E-step, definition of M-step, relationship to k-means.
- Alternative view of EM: expected complete data log-likelihood:



- E-step: Compute posterior over latent variables: $p(Z|X,\theta^{old})$.
- M-step: Find the new estimate of parameters θ^{new} :

$$\theta^{new} = \arg \max_{\theta} \mathcal{Q}(\theta, \theta^{old}).$$

where

$$Q(\theta, \theta^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \ln p(\mathbf{X}, \mathbf{Z}|\theta).$$

- Continuous latent variable models: Probabilistic PCA, Factor Analysis
- PCA, PCA for high-dimensional data
- Probabilistic PCA: definition of probabilistic model, Joint/Marginal density, posterior over latent variables, relationship to standard PCA, EM for PPCA.
- Probabilistic PCA: Maximum likelihood estimation, zero noise limit.
- Factor analysis, definition, marginal/joint/posterior. Relationship to PPCA.



- Sequential data: Markov models, maximum likelihood estimation
- State Space models: definition, transition model, observation model.



- Hidden Markov models: definition, transition model, observation model.
- Maximum likelihood estimation for HMMs, basics of EM algorithm.
- Basics of EM algorithm for HMMs: interring posterior over latent paths and parameter estimation for the transition and observation model.
- Dynamic programming (understanding of alpha-beta recursions)
- Viterbi decoding.