Brain-like Computing
&
Machine Intelligence

Model Inference and Averaging

Dept. Computer Science & Engineering
Shanghai Jiao Tong University

Contents

Course CS &30... SJTU Statistical Learning theory & Application

OBE of The Chapter

- To understand the relations between bootstrap and MLE
- To understand the basic concept of MLE, and grasp the technical implementation of MLE
- To master theoretical issues on MLE
  - Convergence, Convergent rate, Advantages
- To understand the formulation & implementation of Bayesians
- To grasp the formulation EM algorithm
  - Convergence and Implementation

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Bootstrap by Basis Expansions

- Consider a linear expansion $$\mu(x) = \sum_{j=1}^{N} \beta_j h_j(x)$$
- The least square error solution $$\hat{\beta} = (H^T H)^{-1} H^T y$$
- The Covariance of β

$$cor(\hat{\beta}) = (H^T H)^{-1} \hat{\sigma}^2; \qquad \hat{\sigma}^2 = \sum (y_i - \hat{\mu}(x_i))^2 / N$$

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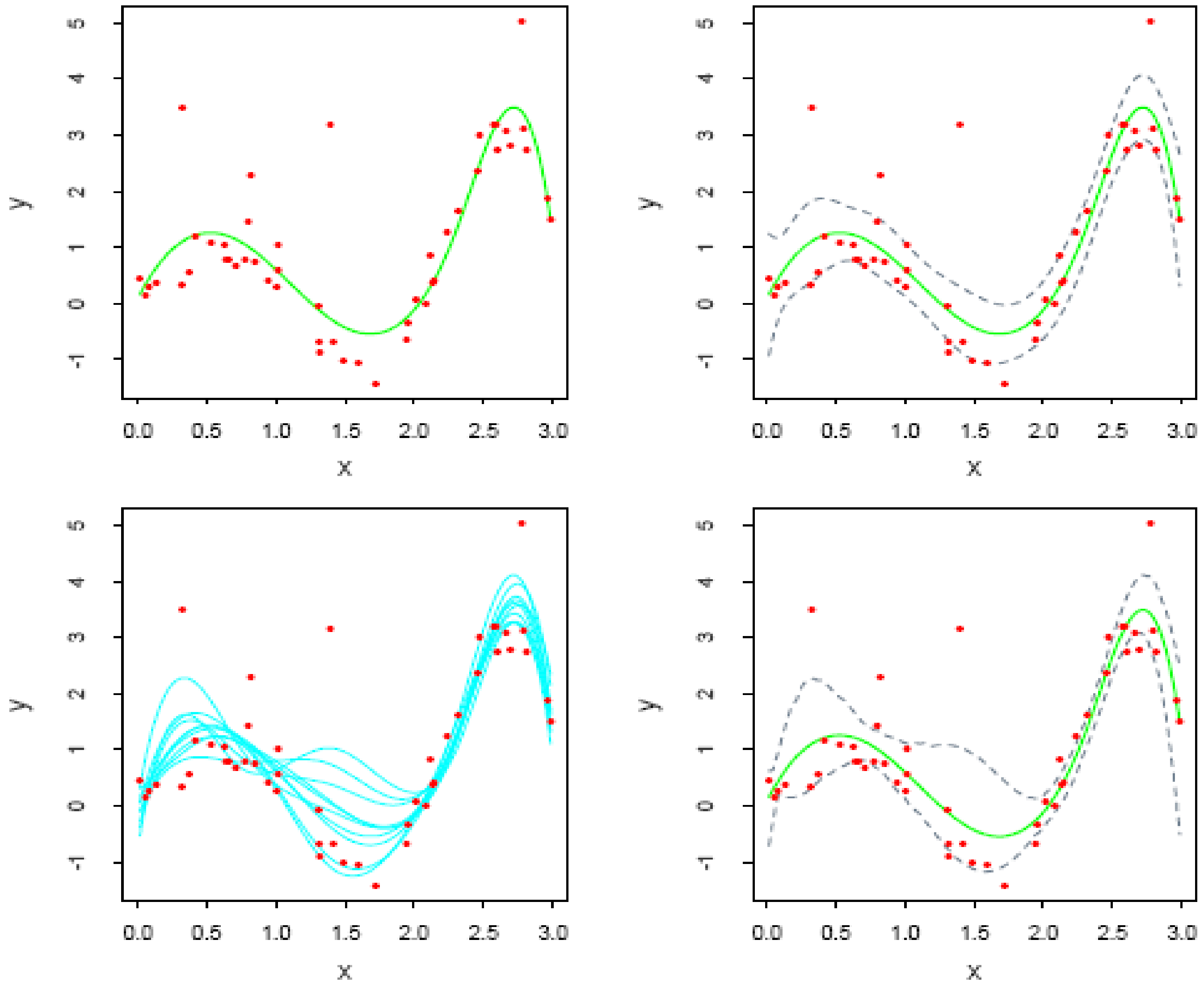

FIGURE 8.2. *(Top left:) B-spline smooth of data. (Top right:) B-spline smooth plus and minus 1.96× standard error bands. (Bottom left:) Ten bootstrap replicates of the B-spline smooth. (Bottom right:) B-spline smooth with 95% standard error bands computed from the bootstrap distribution.*

nd Averaging

Parametric Model

- Assume a parameterized probability density (parametric model) for observations

$$z_i \sim g_\theta(z)$$

E.g. normal distribution $\theta = (\mu, \sigma^2)$; $g_\theta(z) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(z-\mu)^2/\sigma^2}$

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Maximum Likelihood Inference

- Suppose we are trying to measure the true value of some quantity (x_T).
  - We make repeated measurements of this quantity $\{x_1, x_2, \ldots, x_n\}$.
  - The standard way to estimate x_T from our measurements is to calculate the mean value:

$$\mu_x = \frac{1}{N}\sum_{i=1}^{N} x_i$$

and set $x_T = \mu_x$.

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Maximum Likelihood Inference

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DOES THIS PROCEDURE MAKE SENSE?

The maximum likelihood method (MLM) answers this question and provides a general method for estimating parameters of interest from data.

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The Maximum Likelihood Method

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- Statement of the Maximum Likelihood Method
  - Assume we have made N measurements of x: $\{x_1, x_2, \ldots, x_n\}$
  - Assume we know the probability distribution function that describes x: $f(x, a)$.
  - Assume we want to determine the parameter α.
- MLM: pick α to maximize the probability of getting the measurements !

$$L = f(x_1,\alpha)dx \cdot f(x_2,\alpha)dx \cdots f(x_n,\alpha)dx$$

$$= f(x_1,\alpha) \cdot f(x_2,\alpha) \cdots f(x_n,\alpha)[dx^n]$$

$L(\alpha)$ is called $\boxed{\text{the Likelihood Function:}}$ $\quad L(\alpha) = \prod_{i=1}^{N} f(x_i,\alpha)$

Log Maximum Likelihood Method

- Maximizes $L(\alpha)$ by solving the following equation

$$\left.\frac{\partial L(\alpha)}{\partial \alpha}\right|_{\alpha=\alpha^*} = 0$$

  - Often easier to maximize $\ln L(\alpha)$
  - $L(\alpha)$ and $\ln L(\alpha)$ achieve maximum at the same location.

- $\ln L(\alpha)$ converts the product into a summation.

$$\ln L = \sum_{i=1}^{N} \ln f(x_i, \alpha)$$

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Log Maximum Likelihood Method

- The new maximization condition is:

$$\left.\frac{\partial \ln L}{\partial \alpha}\right|_{\alpha=\alpha^*} = \sum_{i=1}^{N} \frac{\partial}{\partial \alpha} \ln f(x_i,\alpha)\Big|_{\alpha=\alpha^*} = 0$$

- Resultant equations: simple linear equations or coupled non-linear equations.

- **Example:** Let $f(x,\alpha)$ be given by a Gaussian distribution function.
- Let $\alpha = \mu$ be the mean of the Gaussian.
- To find the best estimate of α from our set of *n* measurements $\{x_1, x_2, \ldots, x_n\}$.

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An Example: Gaussian

- Gaussian PDF

$$f(x_i,\alpha)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\sum_{i=1}^{n}\frac{(x_i-\alpha)^2}{2\sigma^2}\right)$$

- The likelihood function for this problem is:

$$L=\prod_{i=1}^{n}f(x_i,\alpha)=\prod_{i=1}^{n}\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\sum_{i=1}^{n}\frac{(x_i-\alpha)^2}{2\sigma^2}\right)$$

$$=\left[\frac{1}{\sigma\sqrt{2\pi}}\right]^n e^{-\frac{(x_1-\alpha)^2}{2\sigma^2}}e^{-\frac{(x_2-\alpha)^2}{2\sigma^2}}\cdots e^{-\frac{(x_n-\alpha)^2}{2\sigma^2}}=\left[\frac{1}{\sigma\sqrt{2\pi}}\right]^n e^{-\sum_{i=1}^{n}\frac{(x_i-\alpha)^2}{2\sigma^2}}$$

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An Example: Gaussian

$$\ln L = \ln \prod_{i=1}^{n} f(x_i, \alpha) = \ln\left([\frac{1}{\sigma\sqrt{2\pi}}]^n \exp\left(-\sum_{i=1}^{n} \frac{(x_i - \alpha)^2}{2\sigma^2} \right)\right)$$

$$= n\ln(\frac{1}{\sigma\sqrt{2\pi}}) - \sum_{i=1}^{n} \frac{(x_i - \alpha)^2}{2\sigma^2}$$

- We want to find the *a* that maximizes the log likelihood function:

$$\frac{\partial \ln L}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left[n\ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \sum_{i=1}^{n} \frac{(x_i - \alpha)^2}{2\sigma^2} \right] = 0$$

$$\frac{\partial}{\partial \alpha}\sum_{i=1}^{n}(x_i - \alpha)^2 = 0; \qquad \sum_{i=1}^{n} 2(x_i - \alpha)(-1) = 0 \quad \alpha = \frac{1}{n}\sum_{i=1}^{n} x_i$$

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An Example: Poisson

- Let $f(x,\alpha)$ be given by a Poisson distribution.
- Let α be the mean of the Poisson.
- We want the best estimate of *a* from our set of *n* measurements $\{x_1, x_2, \ldots, x_n\}$
- Poisson PDF:

$$f(x,\alpha) = \frac{e^{-\alpha}\alpha^x}{x!}$$

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An Example: Poisson

- The likelihood function for this problem is:

$$L(\alpha) = \prod_{i=1}^{n} f(x_i, \alpha) = \prod_{i=1}^{n} \frac{e^{-\alpha} \alpha^{x_i}}{x_i !} = \frac{e^{-n\alpha} \alpha^{\sum_{i=1}^{n} x_i}}{x_1 ! x_2 ! .. x_n !}$$

$$\frac{d \ln L}{d\alpha} = \frac{d}{d\alpha}\left(-n\alpha + \ln \alpha \cdot \sum_{i=1}^{n} x_i - \ln(x_1 ! x_2 ! .. x_n !) \right) = -n + \frac{1}{\alpha} \sum_{i=1}^{n} x_i = 0$$

$$\alpha = \frac{1}{n} \sum_{i=1}^{n} x_i$$

Average

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General properties of MLM

- For large data samples (large *n*) the likelihood function, *L*, approaches a Gaussian distribution.
- Maximum likelihood estimates are usually *consistent*.
  - For large *n* the estimates converge to the true value of the parameters we wish to determine.
- Maximum likelihood estimates are usually *unbiased*.
  - For all sample sizes the parameter of interest is calculated correctly.

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General properties of MLM

- Maximum likelihood estimate is *efficient*: the estimate has the smallest variance.
- Maximum likelihood estimate is *sufficient*: it uses all the information in the observations (the x_i's).
- The solution from MLM is unique.
- Bad news: we must know the correct probability distribution for the problem at hand!

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Maximum Likelihood

- We maximize the likelihood function $$L(\theta; \mathbf{Z}) = \prod_{i=1}^{N} g_\theta(z_i)$$
- Log-likelihood function $$\ell(\theta; \mathbf{Z}) = \sum_{i=1}^{N} \log g_\theta(z_i) = \sum_{i=1}^{N} \ell(\theta; z_i)$$
- Estimate θ using the **score function**

$$\dot{\ell}(\theta; \mathbf{Z}) = \sum_{i=1}^{N} \dot{\ell}(\theta; z_i), \qquad \text{where } \dot{\ell}(\theta; z_i) = \frac{\partial \ell(\theta; z_i)}{\partial \theta}$$

- Assume that L takes its maximum in the interior parameter space. Then

$$\dot{\ell}(\hat{\theta}; \mathbf{Z}) = 0$$

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Fisher Information

- Negative sum of second derivatives is the information matrix

$$\mathbf{I}(\theta) = -\sum_{i=1}^{N} \frac{\partial^2 \ell(\theta; z_i)}{\partial\theta\partial\theta^T}$$

is called the observed information, should be greater 0.

- Fisher information (expected information) is

$$\mathbf{i}(\theta) = E_\theta\left[\mathbf{I}(\theta)\right]$$

Assume that θ_0 is the true value of θ

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Sampling Theory

- Basic result of sampling theory
- The sampling distribution of the max-likelihood estimator approaches the following normal distribution, as $N \to \infty$

$$\hat{\theta} \to N(\theta_0, \mathbf{i}(\theta_0)^{-1})$$

when we sample independently from $g_{\theta_0}(z)$

- This suggests to approximate the distribution with

$$N(\hat{\theta}, \mathbf{i}(\hat{\theta})^{-1})$$

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Error Bound

- The corresponding error estimates are obtained from

$$\sqrt{\mathbf{i}(\hat{\theta})^{-1}_{jj}} \quad \text{and} \quad \sqrt{\mathbf{I}(\hat{\theta})^{-1}_{jj}}$$

- The confidence points have the form

$$\hat{\theta}_j - z^{(1-\alpha)} \cdot \sqrt{\mathbf{i}(\hat{\theta})^{-1}_{jj}}$$

$$\text{and} \quad \hat{\theta}_j - z^{(1-\alpha)} \cdot \sqrt{\mathbf{I}(\hat{\theta})^{-1}_{jj}}$$

$z^{(1-\alpha)}$ is the 1-α percentile of the normal distribution

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Approximate form of the Fisher information

- The Fisher information equals

$$I(\theta) = -\mathrm{E}\left[\frac{\partial^2 \log f(X;\theta)}{\partial\theta^2}\right]$$

- The Cramér–Rao bound can then be written as

$$\operatorname{var}(\hat{\theta}) \geq \frac{1}{I(\theta)} = \frac{1}{-\mathrm{E}\left[\frac{\partial^2 \log f(X;\theta)}{\partial\theta^2}\right]}$$

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Contents

- The Bootstrap and Maximum Likelihood Methods
  - Basic theory on MLE (Convergence, Lower bound)
  - Typical Example: regression model
- Bayesian Methods
- The EM Algorithm
- MCMC for Sampling from the Posterior
- Model Averaging and Stacking

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An Example

- Consider a linear expansion

$$y = \sum_{j=1}^{N} \beta_j h_j(x) + \varepsilon \qquad\qquad f(\varepsilon, \sigma^2) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{\varepsilon^2}{2\sigma^2}}$$

- The log-likelihood

$$l(\theta) = -\frac{N}{2} \log \sigma^2 2\pi - \boxed{\frac{1}{2\sigma^2} \sum_{i=1}^{N} \left(y_i - \beta^T h(x_i) \right)^2}$$

- Estimating equations:

$$\frac{\partial l(\theta)}{\partial \beta} = 0; \qquad \frac{\partial l(\theta)}{\partial \sigma^2} = 0.$$

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An Example

- Consider a linear expansion

$$\mu(x)=\sum_{j=1}^{N}\beta_j h_j(x)$$

- The least square error solution

$$\hat{\beta}=(H^T H)^{-1}H^T y$$

- The Covariance of $\hat{\beta}$

$$cor(\hat{\beta})=(H^T H)^{-1}\hat{\sigma}^2; \qquad \hat{\sigma}^2=\sum(y_i-\hat{\mu}(x_i))^2/N$$

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An Example

Consider prediction model $\hat{\mu}(x) = \sum_{j=1}^{N} \hat{\beta}_j h_j(x),$

The standard deviation

$$se[\hat{\mu}(x)] = [h(x)^T (H^T H)^{-1} h(x)]^{1/2} \hat{\sigma}$$

- The confidence region

$$\hat{\mu}(x) \pm 1.96 se[\hat{\mu}(x)]$$

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Contents

- The Bootstrap and Maximum Likelihood Methods
- **Bayesian Methods**
  - How to update pdf after seeing the data and use the prior
- The EM Algorithm
- MCMC for Sampling from the Posterior
- Model Averaging and Stacking

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Bayesian Methods

- Given a sampling model $\Pr(\mathbf{Z}|\theta)$ and a prior $\Pr(\theta)$ for the parameters, estimate the posterior probability

$$\Pr(\theta|\mathbf{Z}) = \frac{\Pr(\mathbf{Z}|\theta)\cdot\Pr(\theta)}{\int \Pr(\mathbf{Z}|\theta)\cdot\Pr(\theta)d\theta}$$

- By drawing samples or estimating its mean or parameters
- Differences to mere counting (frequentist approach)
  - Prior: allow for uncertainties present before seeing the data
  - Posterior: allow for uncertainties present after seeing the data

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Bayesian Methods

- The posterior distribution affords also a predictive distribution of seeing future values z^{new}

$$\Pr\left(z^{\text{new}} \middle| \mathbf{Z}\right) = \int \Pr\left(z^{\text{new}} \middle| \theta\right) \cdot \Pr\left(\theta \middle| \mathbf{Z}\right) d\theta$$

- In contrast, the max-likelihood approach would predict future data on the basis of not accounting for the uncertainty in the parameters $\Pr\left(z^{\text{new}} \middle| \hat{\theta}\right)$

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An Example

- Consider a linear expansion

$$y = \mu_\beta(x) + \varepsilon = \sum_{j=1}^{N} \beta_j h_j(x) + \varepsilon; \qquad p(\varepsilon) = \frac{1}{(2\pi)^{1/2}\sigma_\varepsilon} \exp(-\tfrac{\varepsilon^2}{2\sigma^2})$$

- The prior probability $\beta \;\propto\; N(0, \tau\,\Sigma)$

- The maximum a posterior

$$p(\beta | y, x) \approx p(\beta)\, p(y \,|\, x, \beta) = N(0, \tau\,\Sigma) N_y(\mu_\beta(x) \,|\, \sigma_\varepsilon^2)$$

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MAP (Maximum A Posterior)

- The posterior distribution for β is also Gaussian, with mean and covariance

$$\mathrm{E}(\beta \mid \mathbf{Z}) = \left(\mathbf{H}^T\mathbf{H} + \frac{\sigma^2}{\tau}\Sigma^{-1}\right)^{-1}\mathbf{H}^T\mathrm{y}, \qquad \mathrm{cov}(\beta \mid \mathbf{Z}) = \left(\mathbf{H}^T\mathbf{H} + \frac{\sigma^2}{\tau}\Sigma^{-1}\right)^{-1}\sigma^2.$$

- The corresponding posterior values for $\mu(x) = \sum_{j=1}^{N}\beta_j h_j(x)$

$$\mathrm{E}(\mu(x) \mid \mathbf{Z}) = h(x)^T\left(\mathbf{H}^T\mathbf{H} + \frac{\sigma^2}{\tau}\Sigma^{-1}\right)^{-1}\mathbf{H}^T\mathrm{Y},$$

$$\mathrm{cov}\left[\mu(x), \mu(x') \mid \mathbf{Z}\right] = h(x)^T\left(\mathbf{H}^T\mathbf{H} + \frac{\sigma^2}{\tau}\Sigma^{-1}\right)^{-1}h(x')\sigma^2.$$

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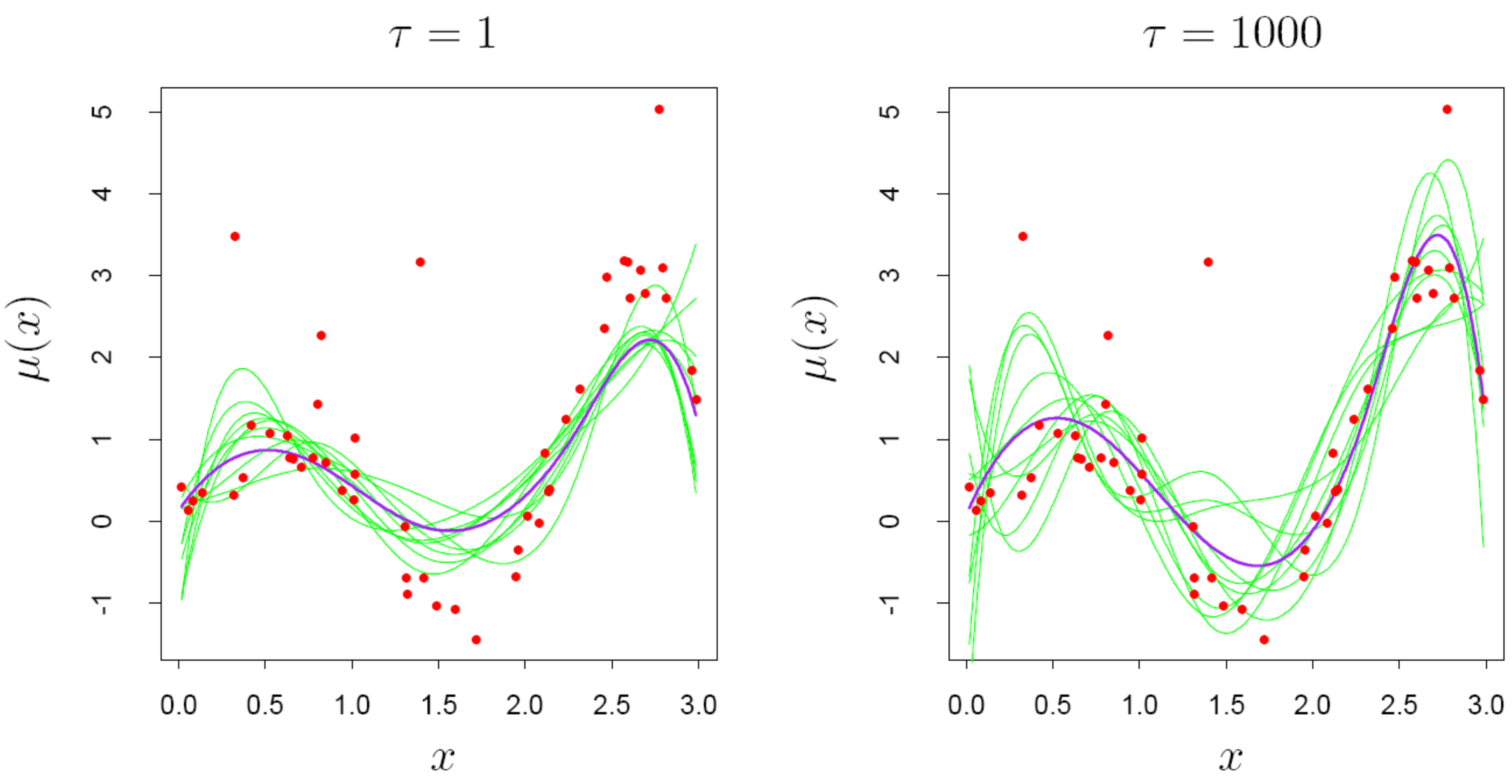

FIGURE 8.4. *Smoothing example: Ten draws from the posterior distribution for the function $\mu(x)$, for two different values of the prior variance τ. The purple curves are the posterior means.*

Bootstrap vs Bayesian

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- The bootstrap mean is an approximate posterior average
- Simple example:
  - Single observation z drawn from a normal distribution $z \propto N(\theta, 1)$
  - Assume a normal prior for θ : $\theta \propto N(0, \tau)$
  - Resulting posterior distribution

$$\theta | z \propto N\left(\frac{z}{1+1/\tau}, \frac{1}{1+1/\tau}\right)$$

Bootstrap vs Bayesian

- Three ingredients make this work
  - The choice of a noninformative prior for θ
  - The dependence of $\ell(\theta; \mathbf{Z})$ on Z only through the max-likelihood estimate $\hat{\theta}$
  - The symmetry of

$$\ell(\theta; \mathbf{Z}) = \ell(\theta; \hat{\theta})$$

$$\ell(\theta; \hat{\theta}) = \ell(\hat{\theta}; \theta) + \text{constant}.$$

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Bootstrap vs Bayesian

- The bootstrap distribution represents an (approximate) nonparametric, noninformative posterior distribution for our parameter.
- But this bootstrap distribution is obtained painlessly without having to formally specify a prior and without having to sample from the posterior distribution.
- Hence we might think of the bootstrap distribution as a “poor man's” Bayes posterior. By perturbing the data, the bootstrap approximates the Bayesian effect of perturbing the parameters, and is typically much simpler to carry out.

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The EM Algorithm

- Gaussian Mixture Model

$$f(x) = \sum_{m=1}^{M} \alpha_m \phi(x; \mu_m, \Sigma_m)$$

- EM algorithm for 2 Gaussian mixtures
  - Given $x_1, x_2, \ldots, x_n,$ log-likelihood:

$$l(y, \theta) = \sum_{i=1}^{N} \log\left[\alpha \phi_{\theta_1}(x_i) + (1-\alpha)\phi_{\theta_2}(x_i)\right]$$

Bad formulation

  - Suppose we observe Latent Binary

$$L(x, z, \theta) = \sum_{\substack{i=1 \\ z_i=1}}^{N} \log\left[\alpha \varphi_{\theta_1}(x_i)\right] + \sum_{\substack{i=1 \\ z_i=0}}^{N} \log\left[(1-\alpha)\varphi_{\theta_2}(x_i)\right]$$

Good formulation

z such that $z = 1 \Rightarrow x \sim \varphi_{\theta_1}, \quad z = 0 \Rightarrow x \sim \varphi_{\theta_2}$

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The EM Algorithm

- The EM algorithm for two-component Gaussian mixtures
  - Take initial guesses $\hat{\pi}, \hat{\mu}_1, \hat{\theta}_1, \hat{\mu}_2, \hat{\theta}_2$ for the parameters
  - Expectation Step: Compute the responsibilities

$$\hat{\gamma}_i = \frac{\hat{\pi}\phi_{\hat{\theta}_2}(y_i)}{(1-\hat{\pi})\phi_{\hat{\theta}_1}(y_i) + \hat{\pi}\phi_{\hat{\theta}_2}(y_i)}, \quad i = 1, \ldots, N$$

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The EM Algorithm

– Maximization Step: Compute the weighted means and variances

$$\hat{\mu}_1 = \frac{\sum_{i=1}^{N}(1-\hat{\gamma}_i)y_i}{\sum_{i=1}^{N}(1-\hat{\gamma}_i)}, \qquad \hat{\sigma}_1^2 = \frac{\sum_{i=1}^{N}(1-\hat{\gamma}_i)(y_i-\hat{\mu}_1)^2}{\sum_{i=1}^{N}(1-\hat{\gamma}_i)},$$

$$\hat{\mu}_2 = \frac{\sum_{i=1}^{N}\hat{\gamma}_i y_i}{\sum_{i=1}^{N}\hat{\gamma}_i}, \qquad \hat{\sigma}_2^2 = \frac{\sum_{i=1}^{N}\hat{\gamma}_i(y_i-\hat{\mu}_1)^2}{\sum_{i=1}^{N}\hat{\gamma}_i},$$

$$\hat{\pi} = \sum_{i=1}^{N}\hat{\gamma}_i \,/\, N$$

– Iterate 2 and 3 until convergence

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The EM Algorithm in General

- $\mathbf{Z}$ input data, with log-likelihood $\ell(\theta, \mathbf{Z})$
- $\mathbf{Z}^m$ latent data (in our example Δ_i)
- $\mathbf{T} = (\mathbf{Z}, \mathbf{Z}^m)$ complete data with log-likelihood $\ell_0(\theta, \mathbf{T})$

$$\Pr\left(\mathbf{Z}^m \middle| \mathbf{Z}, \theta'\right) = \frac{\Pr\left(\mathbf{Z}^m, \mathbf{Z} \middle| \theta'\right)}{\Pr\left(\mathbf{Z} \middle| \theta'\right)}; \qquad \Pr\left(\mathbf{Z} \middle| \theta'\right) = \frac{\Pr\left(\mathbf{T} \middle| \theta'\right)}{\Pr\left(\mathbf{Z}^m \middle| \mathbf{Z}, \theta'\right)}$$

we have $\ell(\theta'; \mathbf{Z}) = \ell_0(\theta'; \mathbf{T}) - \ell_1(\theta'; \mathbf{Z}^m | \mathbf{Z})$

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The EM Algorithm in General

$$\text{we have } \ell(\theta'; \mathbf{Z}) = \ell_0(\theta'; \mathbf{T}) - \ell_1(\theta'; \mathbf{Z}^m \,|\mathbf{Z})$$

- Taking conditional expectations with respect to the distribution of T|Z governed by parameter θ gives

$$\begin{aligned}
\ell(\theta'; \mathbf{Z}) &= \boxed{\int \ell_0(\theta'; \mathbf{T}) \Pr(\mathbf{Z}^m \,|\mathbf{Z}, \theta) d\mathbf{Z}^m} \\
&\quad - \boxed{\int \ell_1(\theta'; \mathbf{Z}^m) \Pr(\mathbf{Z}^m \,|\mathbf{Z}, \theta) d\mathbf{Z}^m} \\
&= \boxed{\mathrm{E}\left(\ell_0(\theta'; \mathbf{T}) \,\middle|\mathbf{Z}, \theta\right)} - \boxed{E\left(\ell_1(\theta'; \mathbf{Z}^m) \,\middle|\mathbf{Z}, \theta\right)} \\
&= Q(\theta'; \theta) - R(\theta'; \theta)
\end{aligned}$$

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The EM Algorithm in General

- Taking conditional expectations with respect to the distribution of T|Z governed by parameter θ gives

$$
\begin{aligned}
R(\theta'; \theta) &= E\left(\ell_1(\theta'; \mathbf{Z}^m \,|\mathbf{Z}) \,\middle|\mathbf{Z}, \theta\right) \\
&= \int \log\left(p(\mathbf{Z}^m \,|\mathbf{Z}, \theta')\right) p(\mathbf{Z}^m \,|\mathbf{Z}, \theta)\, d\mathbf{Z}^m \\
&\leq \int \log\left(p(\mathbf{Z}^m \,|\mathbf{Z}, \theta)\right) p(\mathbf{Z}^m \,|\mathbf{Z}, \theta)\, d\mathbf{Z}^m \\
&= R(\theta; \theta)
\end{aligned}
$$

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Proof of $R(\theta'; \theta) \le R(\theta; \theta)$

If $\phi(x)$ is convex, then $\mathrm{E}[\phi(x)] \ge \phi(E[x])$

$$R(\theta'; \theta) - R(\theta; \theta) =$$

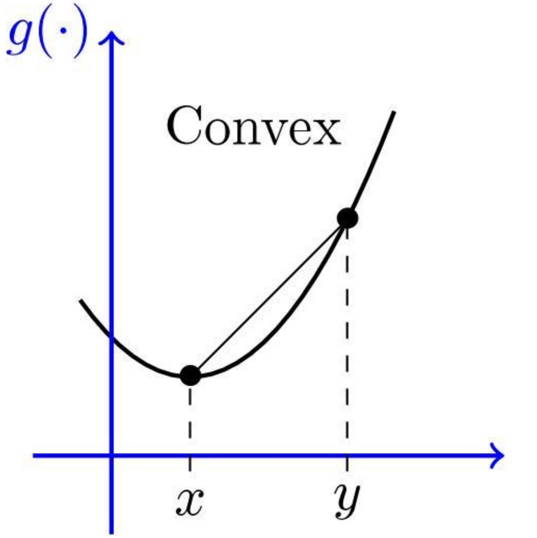
$$= \int [\log(p(\mathbf{Z}^m | \mathbf{Z}, \theta')) - \log(p(\mathbf{Z}^m | \mathbf{Z}, \theta))] p(\mathbf{Z}^m | \mathbf{Z}, \theta)\, d\mathbf{Z}^m$$

$$\le \int \log\left(\frac{p(\mathbf{Z}^m | \mathbf{Z}, \theta')}{p(\mathbf{Z}^m | \mathbf{Z}, \theta)}\right) p(\mathbf{Z}^m | \mathbf{Z}, \theta)\, d\mathbf{Z}^m$$

$$= \mathrm{E}_{p^m}\left[\log\left(\frac{p(\mathbf{Z}^m | \mathbf{Z}, \theta')}{p(\mathbf{Z}^m | \mathbf{Z}, \theta)}\right)\right] \le \log\left[\mathrm{E}_{p^m}\left(\frac{p(\mathbf{Z}^m | \mathbf{Z}, \theta')}{p(\mathbf{Z}^m | \mathbf{Z}, \theta)}\right)\right]$$

$$= \log \int \left(\frac{p(\mathbf{Z}^m | \mathbf{Z}, \theta')}{p(\mathbf{Z}^m | \mathbf{Z}, \theta)}\right) p(\mathbf{Z}^m | \mathbf{Z}, \theta)\, d\mathbf{Z}^m$$

$$= \log \int p(\mathbf{Z}^m | \mathbf{Z}, \theta')\, d\mathbf{Z}^m = \log(1) = 0$$



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The EM Algorithm in General

In the M step, the EM algorithm maximizes $Q(\theta', \theta)$ over θ′, rather than the actual objective function .

$$\ell(\theta'; \mathbf{Z}) = \mathrm{E}\left(\ell_0(\theta'; \mathbf{T}) \middle| Z, \theta\right) - E\left(\ell_1(\theta'; \mathbf{Z}^m | \mathbf{Z}) \middle| Z, \theta\right)$$

$$= Q(\theta'; \theta) - R(\theta'; \theta)$$

$$\ell(\theta'; \mathbf{Z}) - \ell(\theta; \mathbf{Z}) = Q(\theta'; \theta) - Q(\theta; \theta) - \left(R(\theta'; \theta) - R(\theta; \theta)\right) \geq 0$$

Note that $R(\theta*, \theta)$ is the expectation of a log-likelihood of a density (indexed by $\theta*$), with respect to the same density indexed by θ, and hence (by Jensen's inequality) is maximized as a function of $\theta*$, when $\theta* = \theta$

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The EM Algorithm in General

1. Start with initial params $\hat{\theta}$
2. **Expectation Step**: at the j-th step compute

$$Q(\theta', \hat{\theta}^{(j)}) = \mathrm{E}(\ell_0(\theta', \mathbf{T}) \mid \mathbf{Z}, \hat{\theta}^{(j)})$$

   as a function of the dummy argument θ'

3. **Maximization Step**: Determine the new params $\hat{\theta}^{(j+1)}$ by maximizing

$$Q(\theta', \hat{\theta}^{(j)})$$

- Iterate 2 and 3 until convergence

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Contents

- The Bootstrap and Maximum Likelihood Methods
- Bayesian Methods
- Relationship Between the Bootstrap and Bayesian Inference
- **The EM Algorithm**
  - **E-step is expensive in general**
  - **Variational approach; approximation by sampling**
- MCMC for Sampling from the Posterior
- Model Averaging and Stacking

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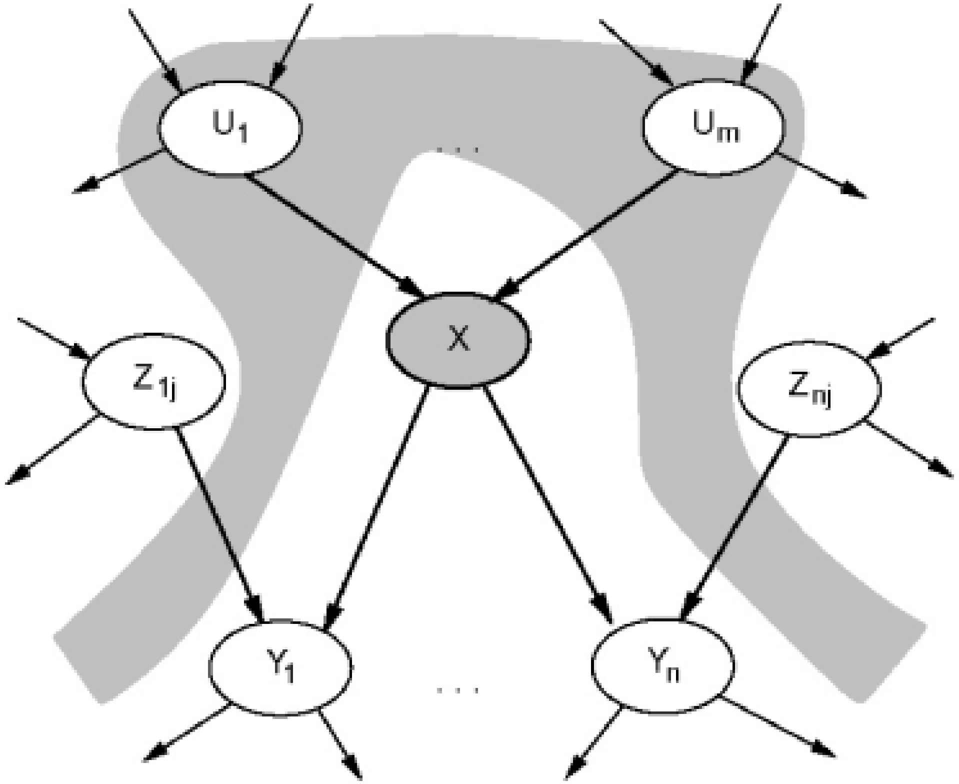
Algorithm 8.3 *Gibbs Sampler.*

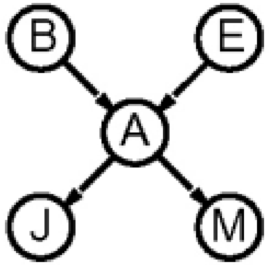
1. Take some initial values $U_k^{(0)}, k = 1, 2, \ldots, K$.
2. Repeat for $t = 1, 2, \ldots, .$:

   For $k = 1, 2, \ldots, K$ generate $U_k^{(t)}$ from
   $\Pr(U_k^{(t)} | U_1^{(t)}, \ldots, U_{k-1}^{(t)}, U_{k+1}^{(t-1)}, \ldots, U_K^{(t-1)})$.
3. Continue step 2 until the joint distribution of $(U_1^{(t)}, U_2^{(t)}, \ldots, U_K^{(t)})$ *does not change.*

Local semantics of Bayesian network

Local semantics: each node is conditionally independent of its nondescendants given its parents

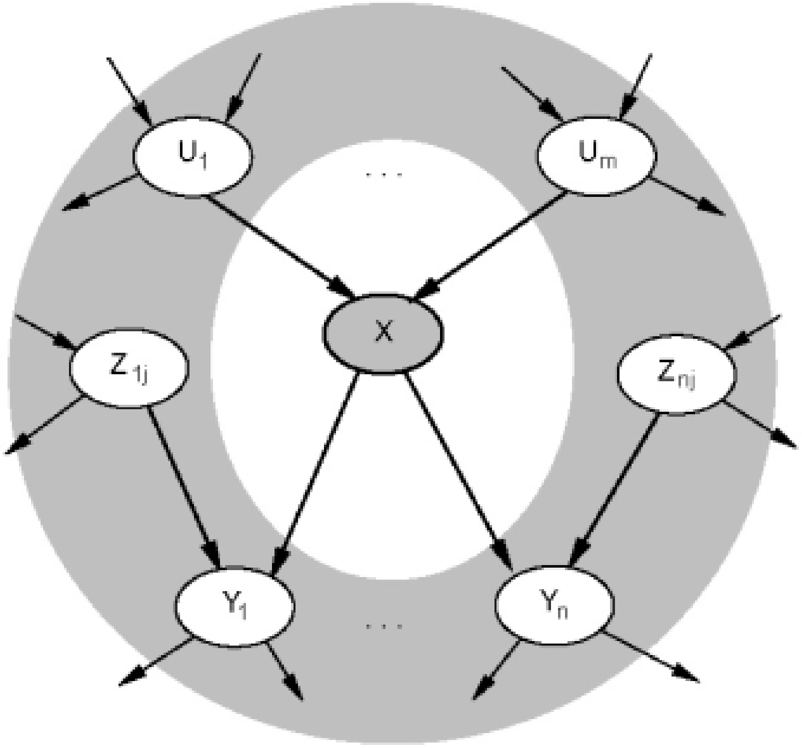


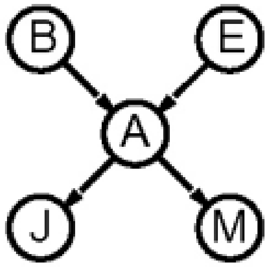


e.g., *JohnCalls* is independent of *Burglary* and *Earthquake*, given the value of *Alarm*.

Markov Blanket

Each node is conditionally independent of all others given its Markov blanket: parents + children + children's parents





e.g., *Burglary* is independent of *JohnCalls* and *MaryCalls* , given the value of *Alarm* and *Earthquake*.

Approximate inference using MCMC*

"State" of network = current assignment to all variables.

Generate next state by sampling one variable given Markov blanket
Sample each variable in turn, keeping evidence fixed

function MCMC-ASK(X, $\mathbf{e}$, bn, N) **returns** an estimate of $P(X|\mathbf{e})$
  local variables: $\mathbf{N}[X]$, a vector of counts over X, initially zero
    $\mathbf{Z}$, the nonevidence variables in bn
    $\mathbf{x}$, the current state of the network, initially copied from $\mathbf{e}$

  initialize $\mathbf{x}$ with random values for the variables in $\mathbf{Y}$
  for $j = 1$ to N **do**
    $\mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1$ where x is the value of X in $\mathbf{x}$
    for each Z_i in $\mathbf{Z}$ **do**
      sample the value of Z_i in $\mathbf{x}$ from $\mathbf{P}(Z_i|MB(Z_i))$ given the values of $MB(Z_i)$ in $\mathbf{x}$
  return NORMALIZE($\mathbf{N}[X]$)

Can also choose a variable to sample at random each time

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Model Averaging and Stacking

- Given predictions $\hat{f}_1(x),\ \hat{f}_2(x), \dots,\ \hat{f}_M(x)$
- Under square-error loss, seek weights

$$\hat{w} = (\hat{w}_1, \hat{w}_2, \dots, \hat{w}_M)$$

- Such that

$$\hat{w} = \arg\min_{w} \mathrm{E}_{\mathcal{P}} \left[Y - \sum_{m=1}^{M} w_m \hat{f}_m(x) \right]^2$$

- Here the input x is fixed and the N observations in Z are distributed according to P

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Model Averaging and Stacking

- The solution is the population linear regression of Y on $\hat{F}(x)^T$, namely

$$\hat{F}(x)^T = \left[\hat{f}_1(x),\ \hat{f}_2(x), \ldots,\ \hat{f}_M(x) \right]$$

- Now the full regression has smaller error, namely

$$\hat{w} = \mathrm{E}_{\mathcal{P}} \left[\hat{F}(x)\hat{F}(x)^T \right]^{-1} \mathrm{E}_{\mathcal{P}} \left[\hat{F}(x)Y \right]$$

- Population linear regression is not available, thus replace it by the linear regression over the training set

$$\mathrm{E}_{\mathcal{P}} \left[Y - \sum_{m=1}^{M} \hat{w}_m \hat{f}_m(x) \right]^2 \leq \mathrm{E}_{\mathcal{P}} \left[Y - \hat{f}_m(x) \right]^2 \quad \forall m$$

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THE END OF TALK