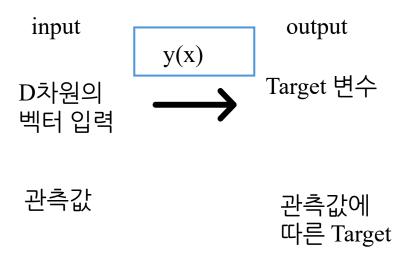
3. Linear Models for Regression

Regression의 목표

- 회귀 모델의 목표 : 입력 값을 통해 예측하는 것
- 선형 회귀 모델의 목표 : 선형 함수 이용

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_D x_D$$

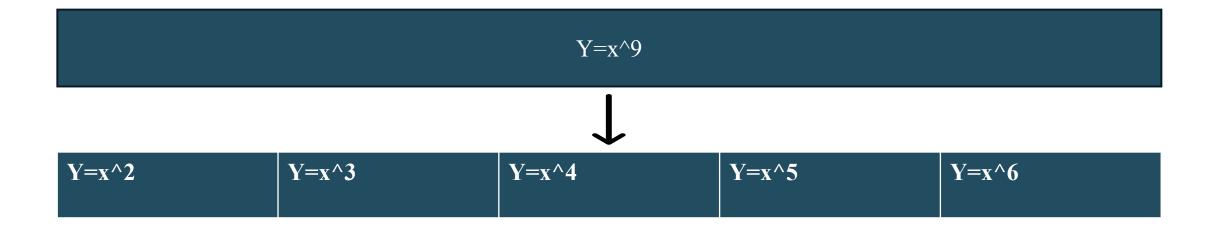
$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) \qquad \phi_0(\mathbf{x}) = 1 \qquad y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x})$$



Polynomial basis function(다항 기저함수)

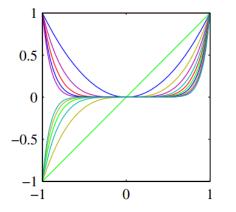
$$\phi_j(x) = x^j$$

Spline function

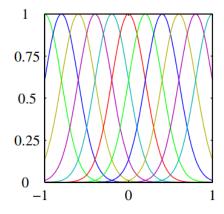


Basis function

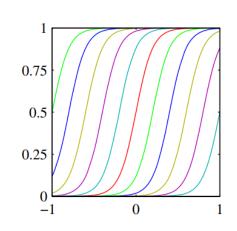
$$\phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$



Polynomial



Gaussian



$$\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

Simoidal basis function

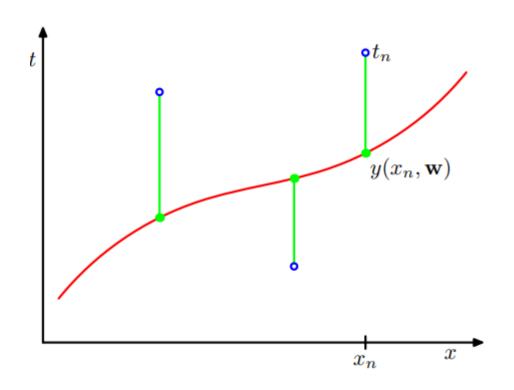
$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

Logistic sigmoid function

$$tanh a = 2\sigma(a) - 1$$

3.1.1 Maximum likelihood and least squares

"가정"



$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon$$
Deterministic function Gause noise

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}).$$

3.1.1 Maximum likelihood and least squares

$$\mathbb{E}[t|\mathbf{x}] = \int tp(t|\mathbf{x}) \, \mathrm{d}t = y(\mathbf{x}, \mathbf{w}).$$
 t의 조건부 평균

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1})$$
 T가 분포에 자체에 영향 받지 않고 독립적으로 추출되었다면...

$$\ln p(\mathbf{t}|\mathbf{w},\beta) = \sum_{n=1}^{N} \ln \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1})$$
$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w}) \quad \text{로그를 취해줌}$$

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\}^2$$
. Error function 정리

3.1.1 Maximum likelihood and least squares

$$\nabla \ln p(\mathbf{t}|\mathbf{w},\beta) = \sum_{n=1}^{N} \left\{ t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) \right\} \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}}.$$

$$0 = \sum_{n=1}^{N} t_n \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} - \mathbf{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_n) \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} \right).$$

$$\mathbf{w}_{\mathrm{ML}} = \left(\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}$$

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - w_0 - \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}_n)\}^2.$$

정리한 결과
$$w_0 = ar{t} - \sum_{j=1}^{M-1} w_j \overline{\phi_j}$$

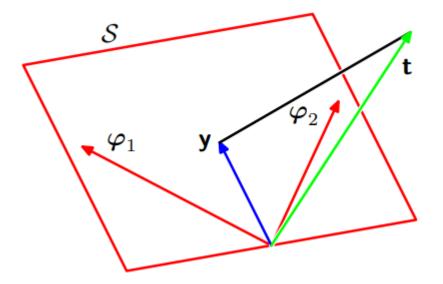
$$\bar{t} = \frac{1}{N} \sum_{n=1}^{N} t_n,$$

$$\bar{t} = \frac{1}{N} \sum_{n=1}^{N} t_n,$$

$$\overline{\phi_j} = \frac{1}{N} \sum_{n=1}^{N} \phi_j(\mathbf{x}_n).$$

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N} \sum_{n=1}^{N} \{t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\}^2$$

3.1.2 Geometry of least squares



3.1.3 Sequential learning

$$\begin{split} y(\mathbf{x},\mathbf{w}) &= w_0 + w_1 x_1 + \ldots + w_D x_D \\ E &= \sum_n E_n, \quad \mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n \\ \mathbf{w}^{(\tau+1)} &= \mathbf{w}^{(\tau)} + \eta (t_n - \mathbf{w}^{(\tau)\mathrm{T}} \boldsymbol{\phi}_n) \boldsymbol{\phi}_n \\ \text{Least mean square(LMS)} \end{split}$$

Stochastic gradient descent : 확률적 경사 하강법 Sequential gradient descent : 순차적 경사 하강법

3.1.4 Regularized least squares

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

$$E_W(\mathbf{w}) = \frac{1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}.$$

$$E_D(\mathbf{w}) \cdot E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\}^2$$

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

$$\mathbf{w} = \left(\lambda \mathbf{I} + \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}.$$

3.1.4 Regularized least squares

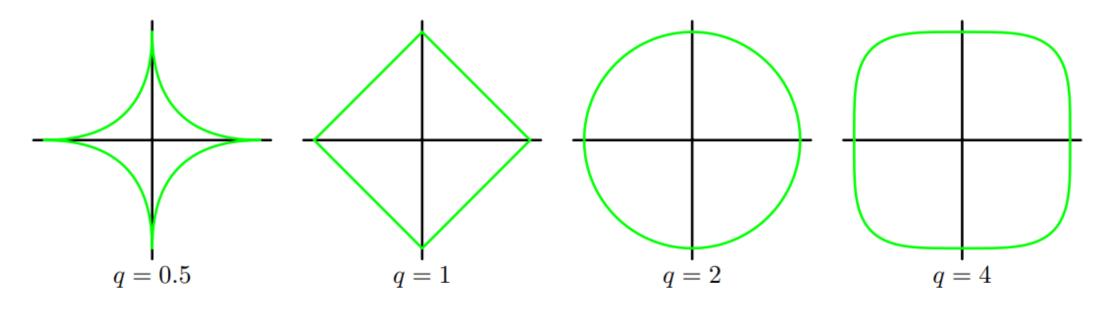


Figure 3.3 Contours of the regularization term in (3.29) for various values of the parameter q.

$$\frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2} \sum_{j=1}^{M} |w_j|^q$$

일반적인 형태의 정규화 항

3.1.5 Multiple outputs

1장

복잡한 모델 \rightarrow 최소 제곱법 이용 시 심각한 overfitting 문제 Basis function을 제한한다면? \rightarrow 모델 유연성에 제약 정규화항 이용 \rightarrow parameter가 많아도 과적합 조절 가능, 하지만 정규화 계수의 값을 적절히 조절할 수 있어야 함.

베이지론 방법론을 바탕으로 각각의 매개변수를 주변화하면 걱정 X 그 전에 빈도주의 관점의 bias variance trade off 살피기

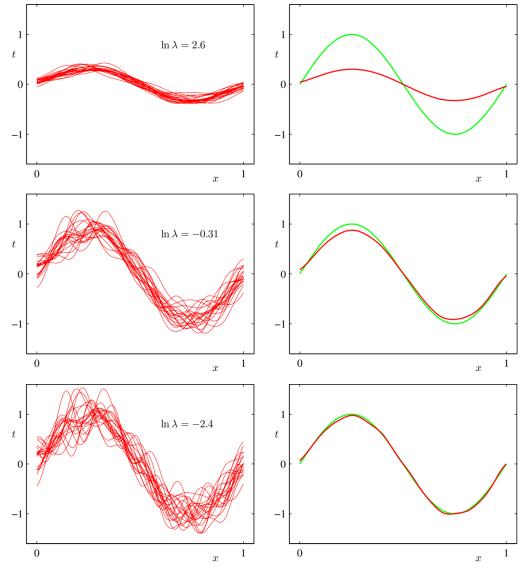
$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x}) d\mathbf{x} + \int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) d\mathbf{x} dt.$$

$$\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2\right] \\ = \underbrace{\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 + \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right]}_{\text{(bias)}^2}.$$
expected loss = (bias)² + variance + noise

$$(\text{bias})^{2} = \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^{2} p(\mathbf{x}) \, d\mathbf{x}$$

$$\text{variance} = \int \mathbb{E}_{\mathcal{D}} \left[\{y(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})]\}^{2} \right] p(\mathbf{x}) \, d\mathbf{x}$$

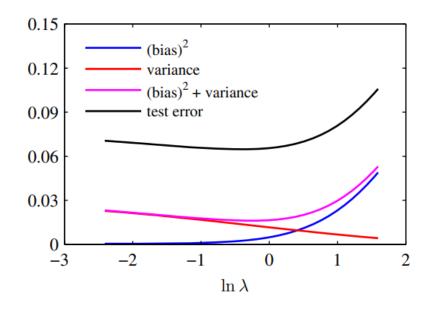
$$\text{noise} = \int \{h(\mathbf{x}) - t\}^{2} p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$



expected loss = $(bias)^2 + variance + noise$

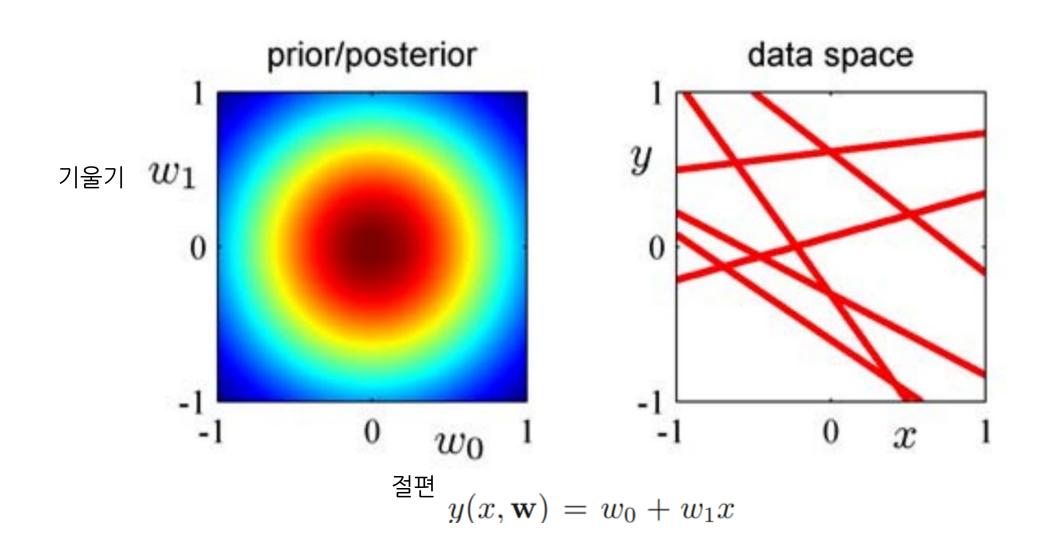
유연한 모델 : bias↓, variance↑

엄격한 모델: bias ↑, variance ↓

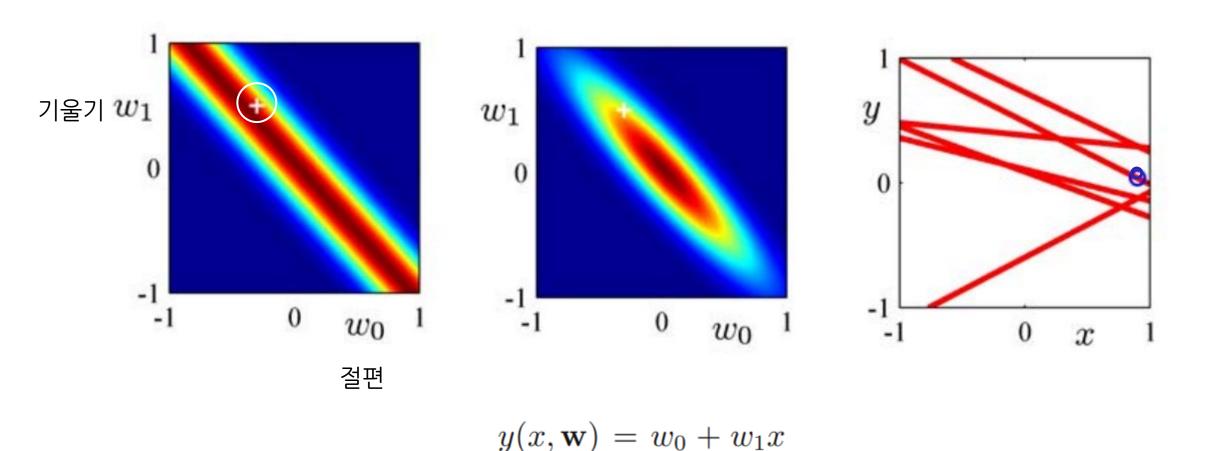


3.3 Bayesian Linear Regression

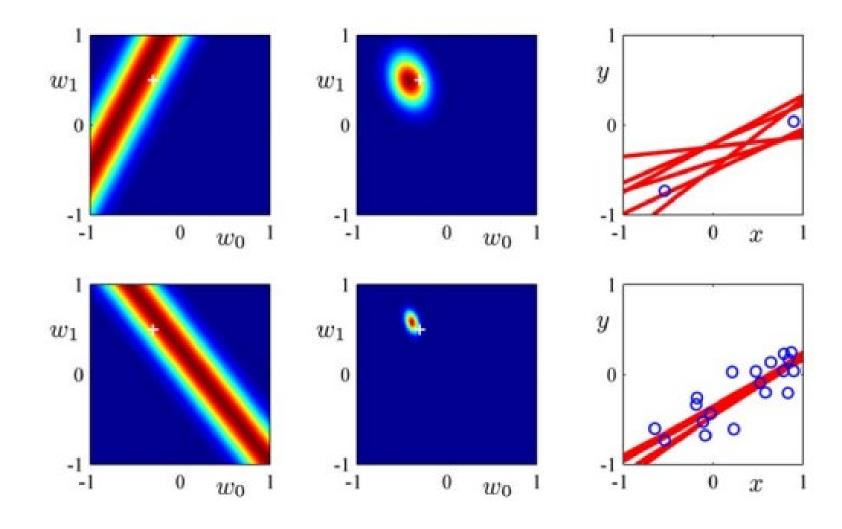
3.3.1 parameter distribution



3.3.1 parameter distribution



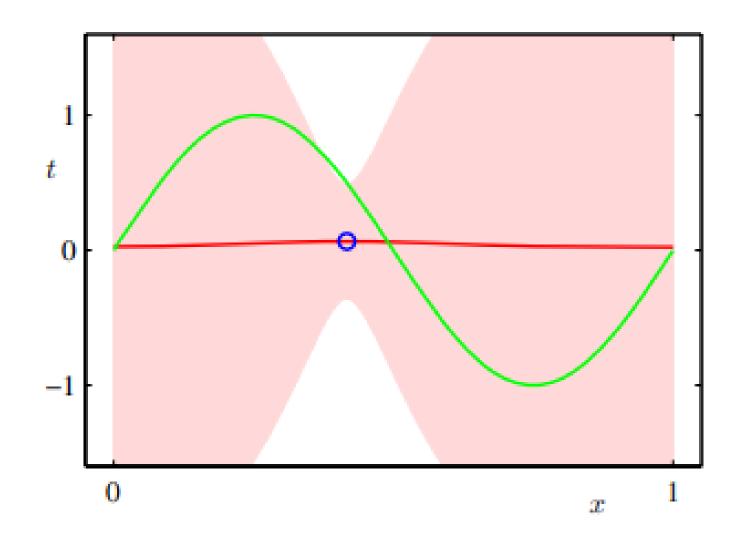
3.3.1 parameter distribution

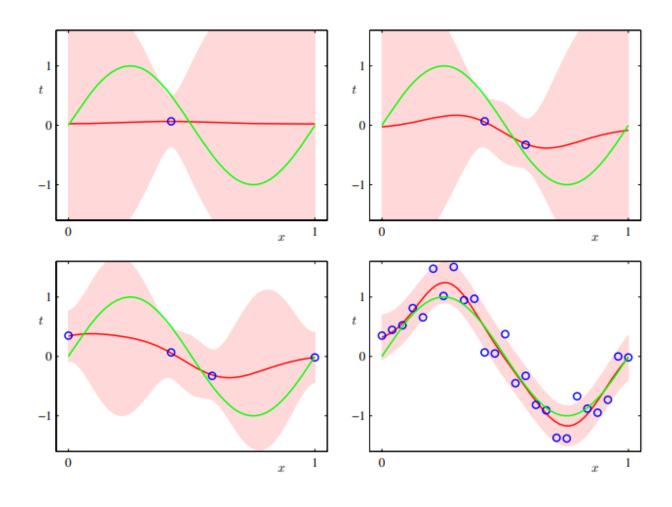


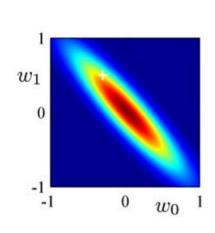
$$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}^{\mathrm{lde}}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

예측 분포

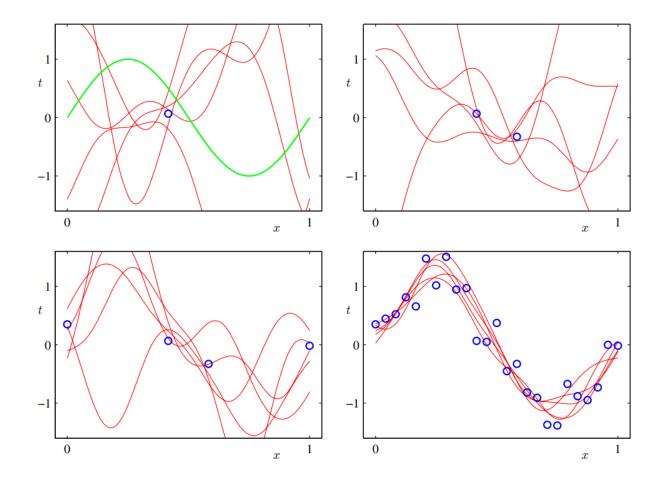
데이터 노이즈
$$\sigma_N^2(\mathbf{x}) = rac{1}{eta} + oldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N oldsymbol{\phi}(\mathbf{x}).$$
예측 분포의 분산 매개변수 w에 대한 불확실성







여기서 뽑은 건 아니 지만 이런 사전/사후 분포에서 뽑아옴

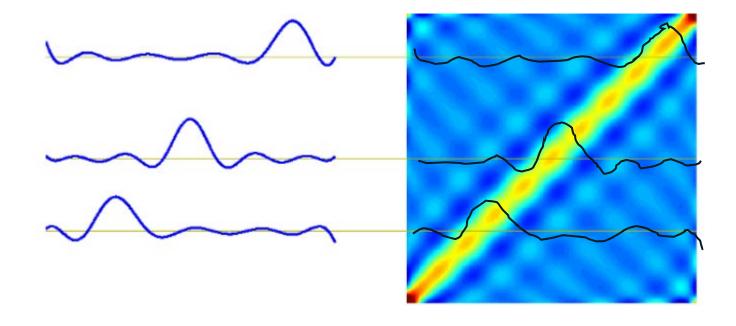


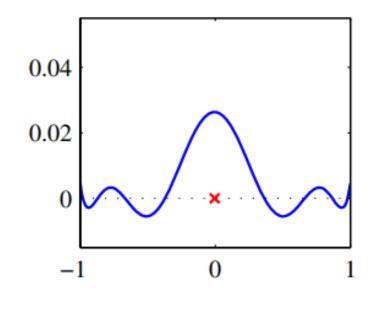
$$y(\mathbf{x}, \mathbf{m}_N) = \mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}) = \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} = \sum_{n=1}^N \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}_n) t_n$$

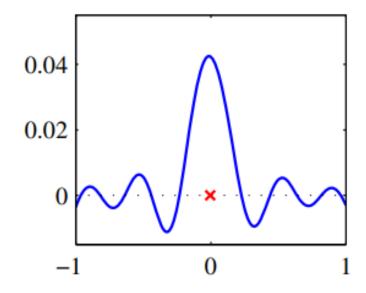
$$y(\mathbf{x}, \mathbf{m}_N) = \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) t_n$$

$$k(\mathbf{x}, \mathbf{x}') = \beta \phi(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \phi(\mathbf{x}')$$

$$k(\mathbf{x}, \mathbf{x}') = \beta \phi(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \phi(\mathbf{x}')$$







다항 기저 함수

시그모이드 기저 함수

$$cov[y(\mathbf{x}), y(\mathbf{x}')] = cov[\phi(\mathbf{x})^{\mathrm{T}}\mathbf{w}, \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}')]$$
$$= \phi(\mathbf{x})^{\mathrm{T}}\mathbf{S}_{N}\phi(\mathbf{x}') = \beta^{-1}k(\mathbf{x}, \mathbf{x}')$$

$$k(\mathbf{x}, \mathbf{z}) = \boldsymbol{\psi}(\mathbf{x})^{\mathrm{T}} \boldsymbol{\psi}(\mathbf{z})$$

where
$$\psi(\mathbf{x}) = \beta^{1/2} \mathbf{S}_N^{1/2} \phi(\mathbf{x})$$



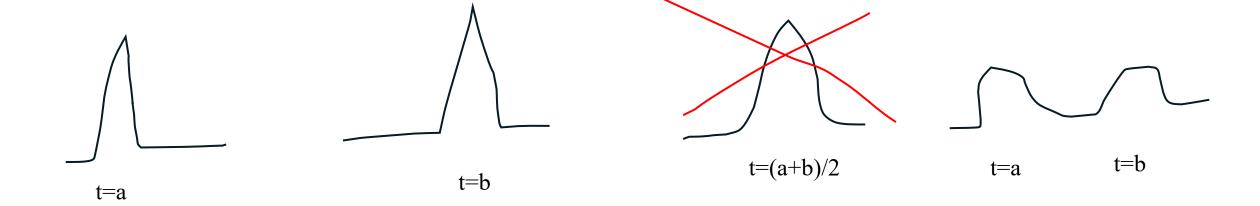
모델 : 관측된 데이터 집합에 대한 확률 분포

$$p(\mathcal{M}_i)$$
 L개의 모델

$$p(\mathcal{M}_i|\mathcal{D}) \propto p(\mathcal{M}_i)p(\mathcal{D}|\mathcal{M}_i).$$
 모델 증거 = 주변 가능도

$$p(\mathcal{D}|\mathcal{M}_i)/p(\mathcal{D}|\mathcal{M}_j)$$
 베이즈 요인

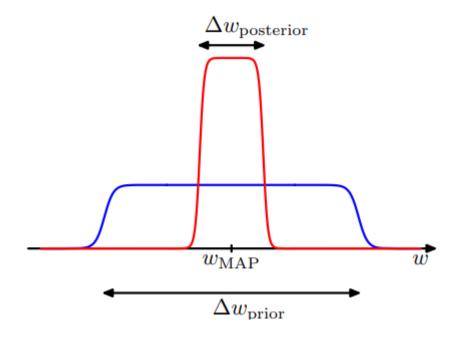
$$p(t|\mathbf{x}, \mathcal{D}) = \sum_{i=1}^{L} p(t|\mathbf{x}, \mathcal{M}_i, \mathcal{D}) p(\mathcal{M}_i|\mathcal{D}).$$



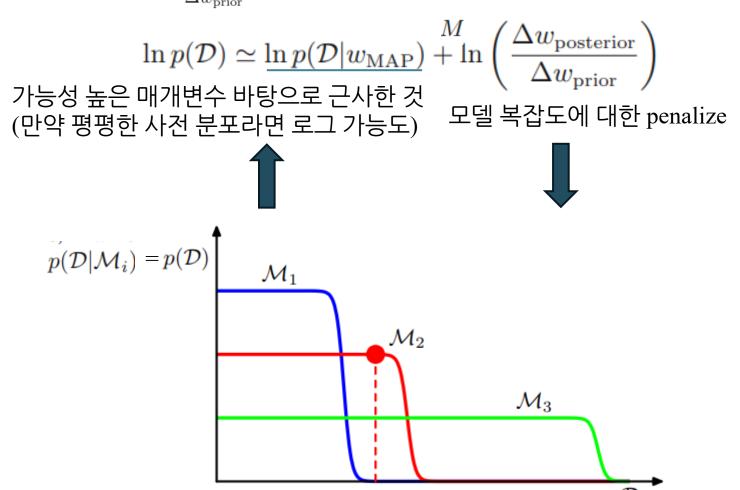
$$p(\mathcal{D}) = \int p(\mathcal{D}|w)p(w) \, \mathrm{d}w \simeq p(\mathcal{D}|w_{\mathrm{MAP}}) \frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}$$

$$\ln p(\mathcal{D}) \simeq \underline{\ln p(\mathcal{D}|w_{\mathrm{MAP}})} + \ln \left(\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}\right)$$

가능성 높은 매개변수 바탕으로 근사한 것 (만약 평평한 사전 분포라면 로그 가능도) 모델 복잡도에 대한 penalize



$$p(\mathcal{D}) = \int p(\mathcal{D}|w)p(w) dw \simeq p(\mathcal{D}|w_{\text{MAP}}) \frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}}$$



 \mathcal{D}_0

매개변수 선택 $p(\mathbf{w})$ \mathbf{J} \mathbf{J} $\mathbf{p}(\mathcal{D}|\mathbf{w})$

데이터 추출

$$p(\mathcal{D}) = \int p(\mathcal{D}|w)p(w) \, \mathrm{d}w \simeq p(\mathcal{D}|w_{\mathrm{MAP}}) \frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}$$

 \mathcal{M}_2

 \mathcal{D}_0

 \mathcal{M}_1

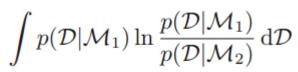
$$\ln p(\mathcal{D}) \simeq \underline{\ln p(\mathcal{D}|w_{\mathrm{MAP}})}^{M} + \ln \left(\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}\right)$$

가능성 높은 매개변수 바탕으로 근사한 것 (만약 평평한 사전 분포라면 로그 가능도)

 \mathcal{M}_3







모델 복잡도에 대한 penalize

매개변수 선택 $p(\mathbf{w})$ \mathbf{J} $\mathbf{p}(\mathcal{D}|\mathbf{w})$

데이터 추출

3.5 The Evidence Approximation

$$p(t|\mathbf{t}) = \iiint p(t|\mathbf{w}, \beta)p(\mathbf{w}|\mathbf{t}, \alpha, \beta)\underline{p(\alpha, \beta|\mathbf{t})} \, d\mathbf{w} \, d\alpha \, d\beta$$

사후 분포

$$p(t|\mathbf{t}) \simeq p(t|\mathbf{t}, \widehat{\alpha}, \widehat{\beta}) = \int p(t|\mathbf{w}, \widehat{\beta}) p(\mathbf{w}|\mathbf{t}, \widehat{\alpha}, \widehat{\beta}) d\mathbf{w}.$$

$$p(\alpha, \beta | \mathbf{t}) \propto p(\mathbf{t} | \alpha, \beta) p(\alpha, \beta)$$

3.5.1Evaluation of the evidence function

가중 매개변수 w에 대해서 적분

$$p(\mathbf{t}|\alpha,\beta) = \int p(\mathbf{t}|\mathbf{w},\beta)p(\mathbf{w}|\alpha)\,\mathrm{d}\mathbf{w}.$$
 주변 가능 도함수
$$p(\mathbf{t}|\alpha,\beta) = \left(\frac{\beta}{2\pi}\right)^{N/2} \left(\frac{\alpha}{2\pi}\right)^{M/2} \int \exp\left\{-E(\mathbf{w})\right\}\,\mathrm{d}\mathbf{w}$$

$$E(\mathbf{w}) = \beta E_D(\mathbf{w}) + \alpha E_W(\mathbf{w})$$

$$= \frac{\beta}{2}\|\mathbf{t} - \Phi \mathbf{w}\|^2 + \frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}.$$

$$E(\mathbf{w}) = E(\mathbf{m}_N) + \frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^{\mathrm{T}}\mathbf{A}(\mathbf{w} - \mathbf{m}_N)$$
 M은 w의 차원수

3.5.1 Evaluation of the evidence function

$$\mathbf{A} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}$$

$$\mathbf{A} = \nabla \nabla E(\mathbf{w})$$

$$\mathbf{m}_N = \beta \mathbf{A}^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}.$$

$$\mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}.$$

$$E(\mathbf{m}_N) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2 + \frac{\alpha}{2} \mathbf{m}_N^{\mathrm{T}} \mathbf{m}_N.$$

$$\int \exp\{-E(\mathbf{w})\} d\mathbf{w}$$

$$= \exp\{-E(\mathbf{m}_N)\} \int \exp\left\{-\frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^{\mathrm{T}} \mathbf{A} (\mathbf{w} - \mathbf{m}_N)\right\} d\mathbf{w}$$

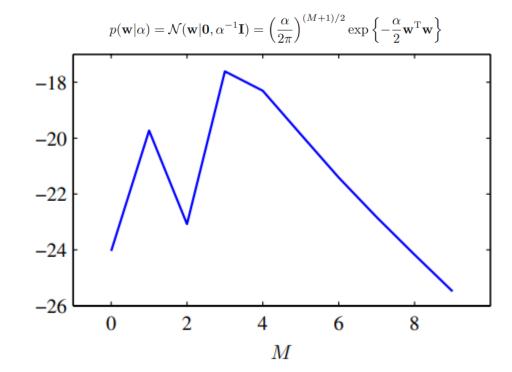
$$= \exp\{-E(\mathbf{m}_N)\} (2\pi)^{M/2} |\mathbf{A}|^{-1/2}.$$

가중 매개변수 w에 대해서 적분

3.5.1 Evaluation of the evidence function

$$\ln p(\mathbf{t}|\alpha,\beta) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - E(\mathbf{m}_N) - \frac{1}{2} \ln |\mathbf{A}| - \frac{N}{2} \ln(2\pi)$$

$$p(\mathbf{t}|\alpha,\beta) = \int p(\mathbf{t}|\mathbf{w},\beta)p(\mathbf{w}|\alpha) d\mathbf{w}.$$



3.5.2 Maximizing the evidence function

가중 매개변수 째에 때빼써 잭뿐

$$p(\mathbf{t}|\alpha,\beta) = \int p(\mathbf{t}|\mathbf{w},\beta)p(\mathbf{w}|\alpha) d\mathbf{w}.$$

$$(\beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}) \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

$$\mathbf{A} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}$$

α에 대해서 미분

$$\ln p(\mathbf{t}|\alpha,\beta) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - E(\mathbf{m}_N) - \frac{1}{2} \ln |\mathbf{A}| - \frac{N}{2} \ln(2\pi)$$

3.5.2 Maximizing the evidence function

$$\alpha \mathbf{m}_N^{\mathrm{T}} \mathbf{m}_N = M - \alpha \sum_i \frac{1}{\lambda_i + \alpha} = \gamma.$$

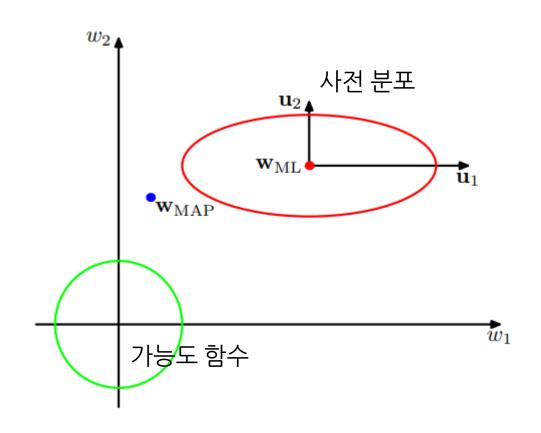
$$\gamma = \sum_{i} \frac{\lambda_i}{\alpha + \lambda_i}.$$

$$\mathbf{m}_N = \beta \mathbf{A}^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}.$$

$$\alpha = \frac{\gamma}{\mathbf{m}_N^{\mathrm{T}} \mathbf{m}_N}.$$

α에 대해서 미분

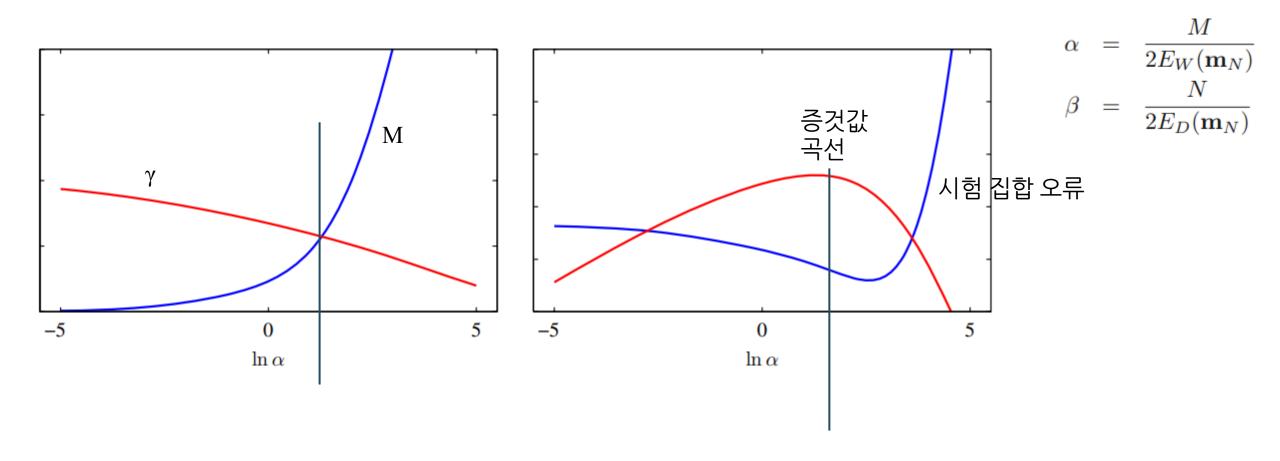
3.5.3 Effective number of parameters



$$\mathbf{m}_N = \beta \mathbf{A}^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}.$$

$$(\beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}) \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

3.5.3 Effective number of parameters



매개변수 선형성 가정

→ 제곱 문제의 해가 닫힌 형태로 존재, 베이지안 과정 통해 풀이 가능

기저 함수 적절히 선택했다면

→ x와 t사이의 비선형성도 모델 가능

선형 모델의 한계점

(해결: 서포트 벡터 머신, 뉴럴 네트워크)

기저 함수가 훈련 데이터 집합 관측 전에 고정

- → 차원의 저주 문제
- → 기저 함수의 숫자는 입력 공간의 차원이 증가함에 따라 빠르게 증가

실제 데이터 집합들의 두 성질 (1)

데이터 벡터들은 보통 내재적 차원수가 입력 공간의 차원수보다 작은 비선형 매니폴드에 근접 가능 → 입력 변수 사이엔 강한 상관관계 존재

방사 기저 함수 네트워크, 서포트 벡터 머신, 상관 벡터 머신 등에서 사용 가능

실제 데이터 집합들의 두 성질(2)

타깃 변수들이 데이터 매니폴드의 몇몇 일부 방향성에 대해서만 중요한 종속성을 가졌을 수 있음

Thank you