

Lecture 6

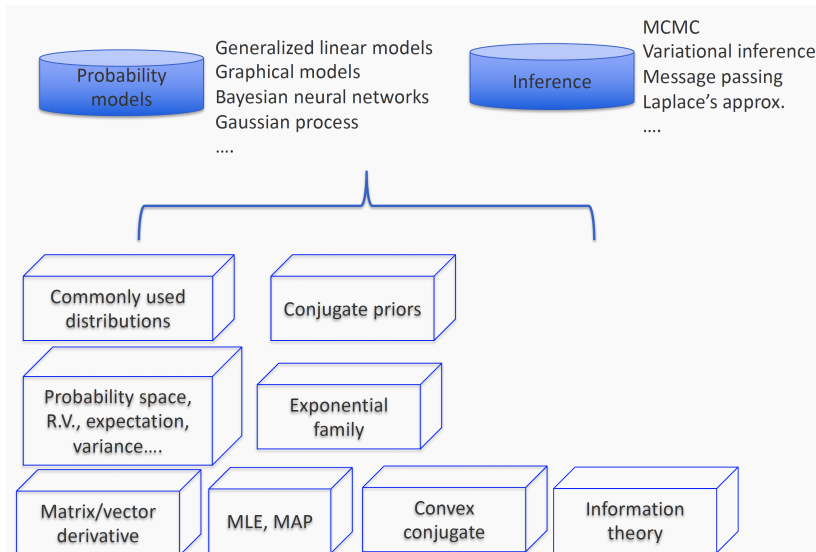
Generalized Linear Models

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- Discuss several important and widely used probabilistic models (and framework)
- Discuss efficient posterior inference algorithm
- We will start with generalized linear models

- Linear models for regression
- Linear models for classification
- Generalized linear models

- Linear models with (nonlinear) basis functions
- Overfitting and regularization
- Bayesian linear regression
- Predictive distribution
- Empirical Bayes

- Simplest model: linear regression

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1x_1 + \dots + w_Dx_D$$

$$\mathbf{x} = (x_1, \dots, x_D)^T$$

- Simplest model: linear regression

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1x_1 + \dots + w_Dx_D$$

$$\mathbf{x} = (x_1, \dots, x_D)^T$$

Limitation: only model linear function of the input variables

- To allow nonlinear modeling, we in general introduce *nonlinear* M basis functions over the input variables

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

- To allow nonlinear modeling, we in general introduce *nonlinear* M basis functions over the input variables

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

$$\phi_j : \mathbb{R}^D \longrightarrow \mathbb{R}$$


Basis function: can be any (nonlinear) over the input variables

- $D = 1$

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

- $D > 1$

$$\phi_j(\mathbf{x}) = x_j \quad \phi_j(\mathbf{x}) = \sin(x_j) \quad \dots$$

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Through nonlinear basis functions, we can model nonlinear functions while maintaining a linear structure

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Through nonlinear basis functions, we can model nonlinear functions while maintaining a linear structure

Neural Networks can be viewed as nonlinear bases as well

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

- Assume the observation is the function corrupted by random Gaussian noise

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

- Consider an observed dataset $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
 $t_1, \dots, t_N$

likelihood

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^N \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1})$$

$$\begin{aligned} \ln p(\mathbf{t}|\mathbf{w}, \beta) &= \sum_{n=1}^N \ln \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}) \\ &= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w}) \end{aligned}$$

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

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


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


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



Design matrix

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

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix} \quad N \times M$$

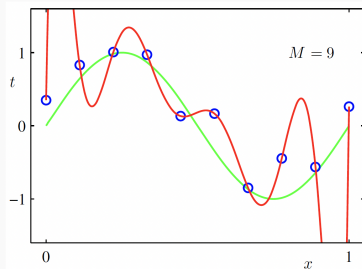
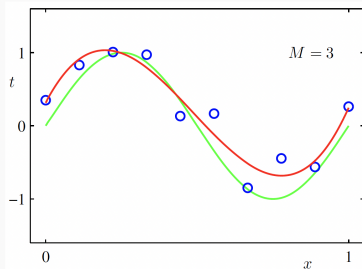
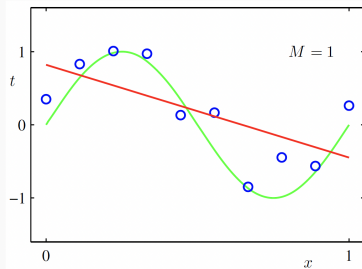
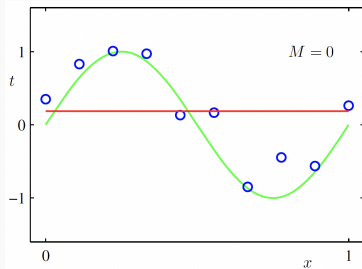
$$\Phi^\dagger \equiv (\Phi^T \Phi)^{-1} \Phi^T \quad \text{Moore-Penrose pseudo-inverse}$$

- Consider polynomial regression

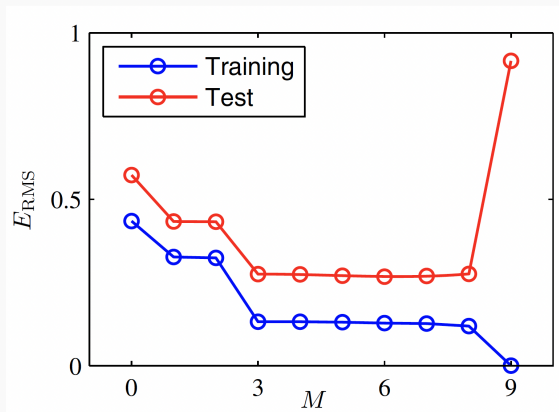
$$y(x, \mathbf{w}) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{j=0}^M w_jx^j$$

Question: what is the highest order we can choose (M)?

Overfitting and Regularization



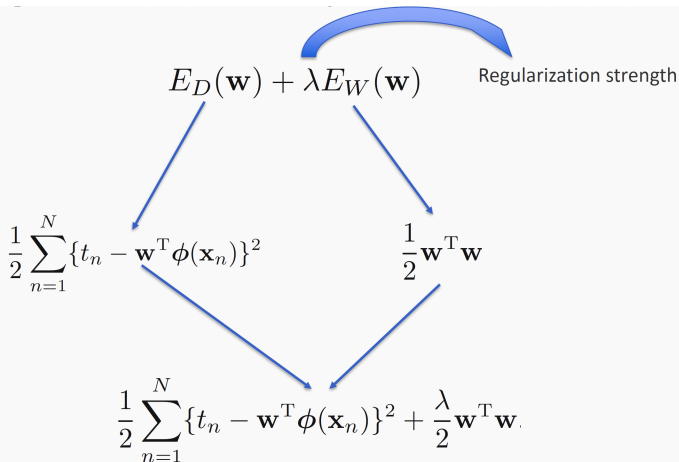
	$M = 0$	$M = 1$	$M = 6$	$M = 9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
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w_9^*				125201.43



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We should constraint the weights from growing too big;

Weights are encouraged to decay toward 0, unless supported by data!



- Set gradient to 0

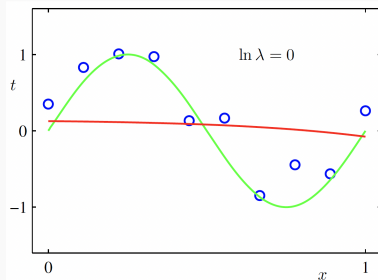
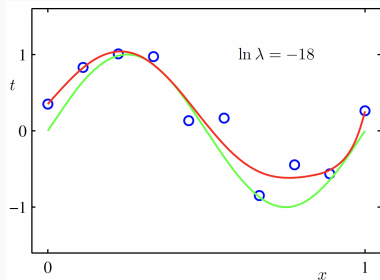
$$\mathbf{w} = (\lambda \mathbf{I} + \Phi^T \Phi)^{-1} \Phi^T \mathbf{t}$$

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

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

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
w_0^*	0.35	0.35	0.13
w_1^*	232.37	4.74	-0.05
w_2^*	-5321.83	-0.77	-0.06
w_3^*	48568.31	-31.97	-0.05
w_4^*	-231639.30	-3.89	-0.03
w_5^*	640042.26	55.28	-0.02
w_6^*	-1061800.52	41.32	-0.01
w_7^*	1042400.18	-45.95	-0.00
w_8^*	-557682.99	-91.53	0.00
w_9^*	125201.43	72.68	0.01

Go Back to Polynomial Regression Again



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

When $q = 2$, we go back to our quadratic regularizer

When $q = 1$, it is known as *lasso*: a classical sparse regression approach; it turns out using lasso can lead many weights to 0

In general, the smaller q leads to sparser models

- We assign a prior over the weights, which corresponds to a regularizer

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{m}_0, \mathbf{S}_0)$$

$$p(\mathbf{t} | \mathbf{w}, \mathbf{X}) = \mathcal{N}(\mathbf{t} | \Phi \mathbf{w}, \beta^{-1} \mathbf{I})$$

$$p(\mathbf{w} | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}_N, \mathbf{S}_N)$$

$$\begin{aligned} \mathbf{m}_N &= \mathbf{S}_N (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \Phi^T \mathbf{t}) \\ \mathbf{S}_N^{-1} &= \mathbf{S}_0^{-1} + \beta \Phi^T \Phi. \end{aligned}$$

- Take a simple choice

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$$

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

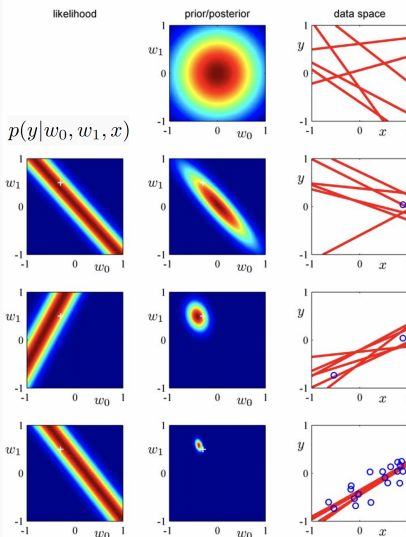
$$\begin{aligned}\mathbf{m}_N &= \beta \mathbf{S}_N \Phi^T \mathbf{t} \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \Phi^T \Phi.\end{aligned}$$

See how the
posterior changes

1st point

2nd point

20th point



- Gaussian prior corresponds to quadratic regularization; Laplace prior lasso
- In general

$$p(\mathbf{w}|\alpha) = \left[\frac{q}{2} \left(\frac{\alpha}{2} \right)^{1/q} \frac{1}{\Gamma(1/q)} \right]^M \exp \left(-\frac{\alpha}{2} \sum_{j=1}^M |w_j|^q \right)$$

q = 1, Laplace's prior

q = 2, Gaussian

- We want to integrate all values of $\mathbf{w}$ into prediction

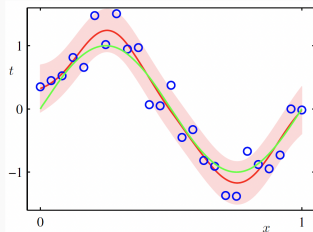
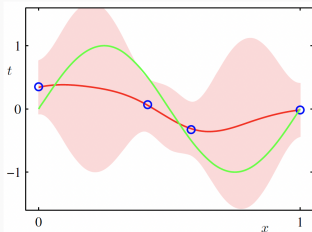
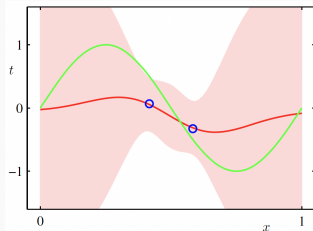
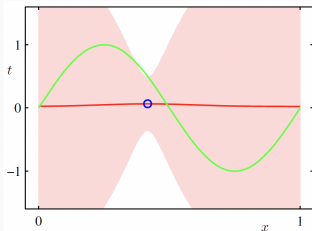
$$p(t|\mathbf{t}, \alpha, \beta) = \int p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) d\mathbf{w}$$

$$\mathcal{N}(t|\mathbf{w}^\top \phi(\mathbf{x}), \beta^{-1})$$

$$\mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

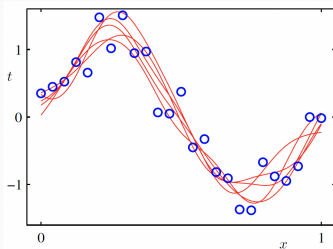
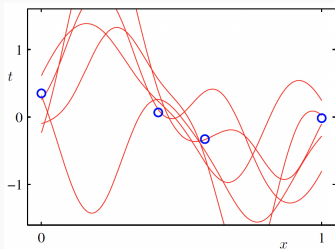
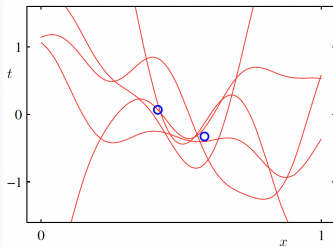
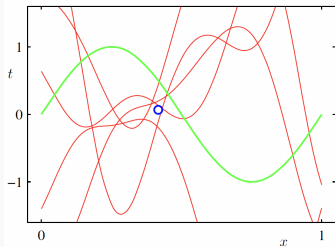
$$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t|\mathbf{m}_N^\top \phi(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \phi(\mathbf{x})^\top \mathbf{S}_N \phi(\mathbf{x})$$



Learn a sinusoidal function with 9 Gaussian basis functions

$t(x, \mathbf{w})$ using samples from the posterior $p(\mathbf{w}|t)$



- Suppose we want to compare a set of models $\{M_1, \dots, M_L\}$.
- The data is generated by one model, which we are not sure. We express the prior by $p(M_i)$
- Given the training data D , we wish to evaluate

$$p(\mathcal{M}_i | \mathcal{D}) \propto p(\mathcal{M}_i) p(\mathcal{D} | \mathcal{M}_i)$$



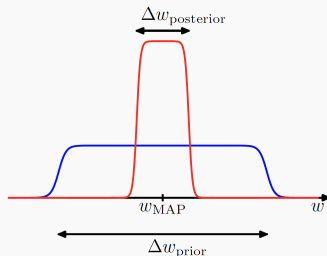
Model evidence

- Bayes factor $p(\mathcal{D}|\mathcal{M}_i)/p(\mathcal{D}|\mathcal{M}_j)$
- Model averaging: Bayesian version of ensemble

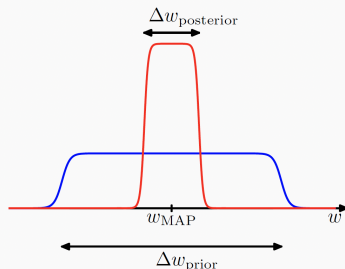
$$p(t|\mathbf{x}, \mathcal{D}) = \sum_{i=1}^L p(t|\mathbf{x}, \mathcal{M}_i, \mathcal{D})p(\mathcal{M}_i|\mathcal{D})$$

- Model selection: choose the most probable model *alone* to make prediction

- Assume the posterior is centered around its mode and flat prior $p(w) = 1/\Delta w_{\text{prior}}$



- Assume the posterior is centered around its mode and flat prior $p(w) = 1/\Delta w_{\text{prior}}$



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

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

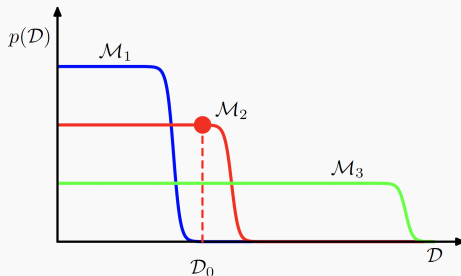
Given M parameters and assume the same ratio

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\mathbf{w}_{\text{MAP}}) + \underbrace{M \ln \left(\frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}} \right)}_{<0}$$

<1

The larger M, the more complex the model, the better fit of the data (1st term), the smaller the second term

- Maximizing evidence naturally leads to a trade-off between data fitting and model complexity



- Approximating the predictive distribution by maximizing the evidence

$$\begin{aligned} p(\mathbf{w}|\alpha) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) \\ p(\mathbf{t}|\mathbf{w}, \mathbf{X}) &= \mathcal{N}(\mathbf{t}|\Phi\mathbf{w}, \beta^{-1}\mathbf{I}) \end{aligned}$$

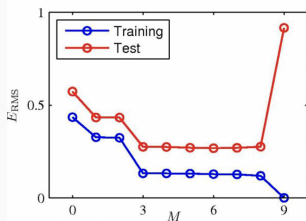
$$p(t|\mathbf{t}) = \iiint p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) p(\alpha, \beta|\mathbf{t}) d\mathbf{w} d\alpha d\beta$$

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

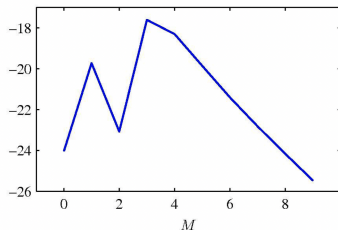
where the hyperparameters $\hat{\alpha}, \hat{\beta}$ are obtained by maximizing the evidence $p(\mathbf{t}|\alpha, \beta)$.

This is known as **Empirical Bayes** or **type II maximum likelihood**

- Consider the degree of polynomial regression



Root-mean-square error



Model evidence

- Linear models for regression
- Linear models for classification
 - Logistic regression
 - Probit regression
 - Multi-class regression
 - Ordinal regression
- General linear models

- Let us first consider binary classification problem: C_1, C_2

$$p(C_1|\phi) = y(\phi) = \sigma(\mathbf{w}^T \phi)$$

$$\sigma(a) = 1/(1 + \exp(-a))$$

Logistic sigmoid function

$$p(C_2|\phi) = 1 - p(C_1|\phi)$$

- Interesting property of sigmoid function

$$\frac{d\sigma}{da} = \sigma(1 - \sigma).$$

- Given a dataset $\{\phi_n, t_n\}$, where $t_n \in \{0, 1\}$, $\phi_n = \phi(\mathbf{x}_n)$ and $n = 1, \dots, N$, the likelihood function is given by

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^N y_n^{t_n} \{1 - y_n\}^{1-t_n}$$

$$\mathbf{t} = (t_1, \dots, t_N)^T$$

$$y_n = p(\mathcal{C}_1|\phi_n) = \sigma(\mathbf{w}^T \phi_n)$$

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}) = -\sum_{n=1}^N \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$



$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \phi_n$$

- Newton-Raphson scheme

$$\mathbf{w}^{(\text{new})} = \mathbf{w}^{(\text{old})} - \mathbf{H}^{-1} \nabla E(\mathbf{w})$$



Hessian matrix

- First consider linear model for regression

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^\top \phi_n\}^2$$

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (\mathbf{w}^\top \phi_n - t_n) \phi_n = \Phi^\top \Phi \mathbf{w} - \Phi^\top \mathbf{t}$$

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (\mathbf{w}^T \phi_n - t_n) \phi_n = \Phi^T \Phi \mathbf{w} - \Phi^T \mathbf{t}$$

$$\mathbf{H} = \nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N \phi_n \phi_n^T = \Phi^T \Phi$$

$$\begin{aligned} \mathbf{w}^{(\text{new})} &= \mathbf{w}^{(\text{old})} - (\Phi^T \Phi)^{-1} \{ \Phi^T \Phi \mathbf{w}^{(\text{old})} - \Phi^T \mathbf{t} \} \\ &= (\Phi^T \Phi)^{-1} \Phi^T \mathbf{t} \end{aligned}$$

The same as least square solution!

One step solves it! Why?

- Logistic regression

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}) = -\sum_{n=1}^N \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \phi_n = \Phi^T (\mathbf{y} - \mathbf{t})$$

$$\mathbf{H} = \nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N y_n (1 - y_n) \phi_n \phi_n^T = \Phi^T \mathbf{R} \Phi$$

N x N diagonal matrix $R_{nn} = y_n(1 - y_n) \quad y_n = \sigma(\mathbf{w}^T \phi_n)$

$$\begin{aligned}\mathbf{w}^{(\text{new})} &= \mathbf{w}^{(\text{old})} - (\Phi^T \mathbf{R} \Phi)^{-1} \Phi^T (\mathbf{y} - \mathbf{t}) \\ &= (\Phi^T \mathbf{R} \Phi)^{-1} \{ \Phi^T \mathbf{R} \Phi \mathbf{w}^{(\text{old})} - \Phi^T (\mathbf{y} - \mathbf{t}) \} \\ &= (\Phi^T \mathbf{R} \Phi)^{-1} \Phi^T \mathbf{R} \mathbf{z}\end{aligned}$$

Iterative updates

$$\mathbf{z} = \underbrace{\Phi \mathbf{w}^{(\text{old})} - \mathbf{R}^{-1} (\mathbf{y} - \mathbf{t})}_{\text{Updated responses}}$$

Updated responses

Weight matrix $\mathbf{R}$ depends on $\mathbf{W}$

- Suppose we have K classes, $C_1, \dots, C_K$

$$p(C_k|\phi) = y_k(\phi) = \frac{\exp(a_k)}{\sum_j \exp(a_j)} \quad a_k = \mathbf{w}_k^T \phi$$

K groups of parameters $\{\mathbf{w}_k\}$

This is often referred to as softmax

$$\frac{\partial y_k}{\partial a_j} = y_k(I_{kj} - y_j)$$

- likelihood

$$p(\mathbf{T}|\mathbf{w}_1, \dots, \mathbf{w}_K) = \prod_{n=1}^N \prod_{k=1}^K p(\mathcal{C}_k | \phi_n)^{t_{nk}} = \prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}$$

$\mathbf{T}$: N x K observation matrix, each row is one-hot vector

- We can use Newton-Raphson updates as well

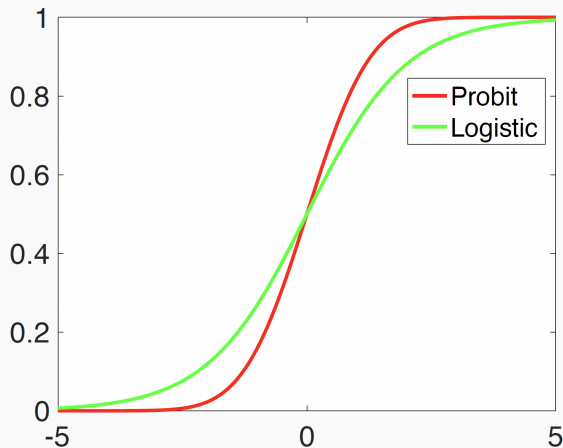
$$\nabla_{\mathbf{w}_j} E(\mathbf{w}_1, \dots, \mathbf{w}_K) = \sum_{n=1}^N (y_{nj} - t_{nj}) \phi_n$$

$$\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_j} E(\mathbf{w}_1, \dots, \mathbf{w}_K) = - \sum_{n=1}^N y_{nk} (I_{kj} - y_{nj}) \phi_n \phi_n^T.$$

- An alternative model for binary classification

$$p(\mathcal{C}_1|\phi) = y(\phi) = \psi(\mathbf{w}^\top \phi)$$

$$\psi(a) = \int_{-\infty}^a \mathcal{N}(x|0, 1)dx$$



- Equivalent latent variable model

$$\text{Given } a = \mathbf{w}^\top \boldsymbol{\phi}$$

sample the label t from $p(t|a) = \psi(a)^t (1 - \psi(a))^{1-t}$



Sample a latent variable z from

$$z \sim \mathcal{N}(z|a, 1)$$

Sample the label t from a step distribution

$$p(t|z) = I(t=0)I(z \leq 0) + I(t=1)I(z \geq 0)$$

- Consider to predict K classes with *ordering* relationship, $C_1 < C_2 < \dots < C_K$, e.g., rank, disease progression, ...
- Using multi-class logistic regression is not appropriate

- Consider multi-class Probit regression

Partition real domain into ordered regions

$$(\infty, b_1], (b_1, b_2], \dots, (b_{K-1}, b_K], (b_K, \infty)$$

$$\text{Given } a = \mathbf{w}^\top \phi$$

Sample a latent variable z from $z \sim \mathcal{N}(z|a, 1)$

Check which region z falls in, e.g., $[b_k, b_{k+1})$

Output the corresponding label: k

- Let us consider the exponential family to model data

$$p(t|\eta) = \exp(\eta t - g(\eta))$$

Consider the expectation of t

$$\mathbb{E}[t|\eta] = y = \frac{dg(\eta)}{d\eta}$$

This is a mapping $\eta = \psi(y)$

From expectation to natural parameters

- In linear model, we commonly model the expectation parameters as

$$y = f(\mathbf{w}^\top \phi(\mathbf{x}))$$

- If we choose $f = \psi^{-1}$ $\eta = \psi(y)$



$$\eta = \psi(\psi^{-1}(\mathbf{w}^\top \phi(\mathbf{x}))) = \mathbf{w}^\top \phi(\mathbf{x})$$

f^{-1} is called link function (link expectation to natural paras)

- Given training data $(\mathbf{x}_1, t_1), \dots, (\mathbf{x}_N, t_N)$

$$\begin{aligned} E(\mathbf{w}) &= \sum_{n=1}^N \log p(t_n | \eta) \\ &= \sum_{n=1}^N \eta_n t_n - g(\eta_n) \end{aligned}$$

$$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \sum_{n=1}^N \frac{\partial \eta_n}{\partial \mathbf{w}} t_n - \frac{\partial g}{\partial \eta_n} \frac{\partial \eta_n}{\partial \mathbf{w}}$$

$$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \sum_{n=1}^N \frac{\partial \eta_n}{\partial \mathbf{w}} t_n - \frac{\partial g}{\partial \eta_n} \frac{\partial \eta_n}{\partial \mathbf{w}}$$

$$= \sum_{n=1}^N \phi(\mathbf{x}_n) (t_n - y_n)$$

Feature vector
prediction error

$$\mathbb{E}[t_n | \eta_n] = y_n = \frac{dg(\eta_n)}{d\eta_n}$$

$$\eta_n = \mathbf{w}^\top \phi(\mathbf{x}_n)$$

This is consistent with linear regression and logistic regression

- What is design matrix?
- How to obtain MLE for linear regression?
- How to obtain posterior and predictive distribution for linear regression?
- What is the empirical Bayes and type II MLE?
- Newton-Rapson method for logistic regression
- What is probit regression? What is the equivalent model? How to conduct multi-class classification?
- What is generalized linear model? What is link function? What is the general form of the gradient?