MAP 534 Introduction to machine learning Linear models for classification II

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Outline

Probabilistic discriminative models for classification

Logistic regression

Bayesian logistic regression

Introduction to classification: setting

- We consider a supervised setting.
- Decide how to encode inputs and outputs: this defines the input space X, and the output space Y.
- Here we consider specifically the classification problem: Y is a finite set,

$$\mathsf{Y} = \{1, \dots \mathsf{K}\}$$
 , in most of this lecture even $\mathsf{Y} = \{0, 1\}$.

• In this lecture, we apply the three machine learning paradigms to address:

$$y_{\text{pred}} = \mathscr{C}(x_{\text{new}})$$
,

and aim to quantify if possible the uncertainties of our predictions.

- Here & is called a classifier.
- Recall that the three paradigms are:
 - deterministic discriminative learning ✓;
 - probabilistic generative learning ✓;
 - ullet probabilistic discriminative learning \Longrightarrow today;

Generative vs discriminative models

• Recall the generative setting: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ are i.i.d observations of random variables (X, Y):

$$X|Y \sim p_w(\cdot|Y)$$
, $Y \sim p_Y$.

We consider here a family of conditional densities

$$\{(x,y)\mapsto p_w(x|y): w\in\Theta\}$$
.

ullet From an estimator \hat{w} , we end up using Bayes formula with the predictive distribution

$$p_{\hat{w}}(y|x_{\text{new}}) = \frac{p_{\hat{w}}(x|y)p_{Y}(y)}{\sum_{y' \in Y} p_{\hat{w}}(x|y')p_{Y}(y')} \propto p_{\hat{w}}(x|y)p_{Y}(y) .$$

 Idea of discriminative models: directly consider a family of conditional distributions

$$\{(y,x)\mapsto p_w(y|x): w\in\Theta\}$$
.

Discriminative models

 Idea of discriminative models: directly consider a family of conditional distributions

$$\{(y,x)\mapsto p_w(y|x): w\in\Theta\}$$
.

• Choosing a prior $p_X(x)$, we get the likelihood

$$L(w; \mathcal{D}) = \prod_{i=1}^{N} \{p_w(y_i|x_i)p_X(x_i)\}.$$

- In most cases, we do not infer/learn p_X .
- Then, w is estimated by maximum likelihood which is equivalent in that case to minimize:

$$E(w) = -\sum_{i=1}^{N} \log p_w(y_i|x_i).$$

• We end up with estimating the predictive probabilities $p_{\tilde{w}}(y|x_{\text{new}})$ and the prediction:

$$y_{\mathsf{pred}} = \operatorname*{argmax}_{y} p_{\hat{w}}(y|x_{\mathsf{new}}) .$$

- Phow to choose the family $\{(y,x)\mapsto p_w(y|x):w\in\Theta\}$?
- We can first take inspiration from the form we obtain in generative models.

Introduction and motivation: logistic and softmax functions

• Recall the generative setting: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ are i.i.d observations of random variables (X, Y):

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ullet In the case $Y=\{0,1\}$, this can be written on the form:

$$p_{\hat{w}}(1|x_{\text{new}}) = \sigma(a(x_{\text{new}}, \hat{w})), \quad \sigma(t) = \frac{e^{t}}{1 + e^{t}}$$
 $a(x_{\text{new}}, w) = \log\left(\frac{p_{w}(x_{\text{new}}|1)p_{\text{prior}}(1)}{p_{w}(x_{\text{new}}|0)p_{\text{prior}}(0)}\right)$

- And similarly for y = 0...
- The quantity a(x, w) is called an activation.
- ullet The function σ is called the logistic sigmoid function.

The logistic sigmoid function

- $\sigma(t)=rac{\mathrm{e}^t}{1+\mathrm{e}^t}$ very important function in ML.
- Some properties:

$$\sigma(-t) = 1 - \sigma(t)$$
, inverse $\sigma \mapsto \log(\sigma/(1-\sigma))$.

Proof.

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Introduction and motivation: logistic and softmax functions

• Recall the generative setting: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ are i.i.d observations of random variables (X, Y):

$$X|Y \sim p_w(\cdot|Y)$$
, $Y \sim p_Y$.

- We consider here a family of conditional densities $\{(x,y)\mapsto p_w(x|y):w\in\Theta\}.$
- \bullet In the case $Y=\{0,1\},$ the predictive probability can be written of the form:

$$\begin{aligned} p_w(1|x_{\text{new}}) &= \sigma(a(x_{\text{new}}, w)) \;, \quad \sigma(t) = \frac{e^t}{1 + e^t} \\ a(x_{\text{new}}, w) &= \log\left(\frac{p_w(x_{\text{new}}|1)p_{\text{prior}}(1)}{p_w(x_{\text{new}}|0)p_{\text{prior}}(0)}\right) \end{aligned}$$

- The activation $a(x_{new}, \hat{w}) = \log \text{ odds} / \log \text{ of ratio of posterior probabilities}$
- The expression for $p_{\hat{w}}$ seems to be overly complicated given the first simple expression given previously...
- However it gives ideas of many discriminative models: choose a!
- Idea of logistic regression: take $a(x_{\text{new}}, w) = \phi(x_{\text{new}})^T w$, linear with respect to the parameter.

Multiclass discrtiminative probabilistic problem

- This generalizes to the multiclass scenario K > 2.
- In that situation: we end up with predictive probabilities for the class k of the form:

$$p_{W}(k|x_{\text{new}}) = \frac{\exp(a(x_{\text{new}}, w_{k}))}{\sum_{j=1}^{K} \exp(a(x_{\text{new}}, w_{j}))},$$

where $W = \{w_j\}_{j=1}^K$ is the parameter to infer.

• The function

$$\boldsymbol{\sigma}: \mathbb{R}^K \to \operatorname{Simplex}_K = \{(\varpi_1, \dots, \varpi_K) \in [0, 1]^K \,:\, \textstyle\sum_{k=1}^K \varpi_k = 1\}:$$

$$\sigma(a_1,\ldots,a_K) = \left(\frac{\mathrm{e}^{a_1}}{\sum_{j=1}^K \mathrm{e}^{a_j}},\ldots,\frac{\mathrm{e}^{a_K}}{\sum_{j=1}^K \mathrm{e}^{a_j}}\right)^{\mathrm{T}}$$

is called the normalized exponential or softmax function.

- With this notation, $p_W(k|x_{\text{new}}) = \sigma(a_1, \dots, a_K)_k$, with $a_k = a(x_{\text{new}}, w_k)$.
- This remark suggests also to directly choose the function $a: X \times \mathbb{R}^d \to \mathbb{R}$.

Outline

Probabilistic discriminative models for classification

Logistic regression

Bayesian logistic regression

Fixed basis functions

- We consider here fixed basis functions $\phi = {\{\phi_j\}_{j=1}^d, \ \phi_j : \mathsf{X} \to \mathbb{R}}$.
- This helps in the process of modeling the predictive distribution from activations.
- Without loss of generality, we then consider that the feature $x_i \in \mathbb{R}^d$ changing $x_i \leftarrow \{\phi_1(x_i), \dots, \phi_d(x_i)\}$.

Logistic regression: likelihood

- We first consider the 0-1 prediction task, $Y = \{0,1\}$.
- ullet We consider here the family of conditional/predictive distributions: $w \in \mathbb{R}^d$.

$$p_{w}(y_{\text{pred}}|x_{\text{new}}) = \sigma(w^{\mathrm{T}}x_{\text{new}})^{y_{\text{pred}}}(1 - \sigma(w^{\mathrm{T}}x_{\text{new}}))^{1 - y_{\text{pred}}} \;, \quad \sigma(t) = \frac{\mathrm{e}^{t}}{1 + \mathrm{e}^{t}} \;.$$

• This corresponds to the statistical model: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ are i.i.d observations from

$$Y|X \sim \text{Ber}(\sigma(w^{T}X))$$
.

• The likelihood is then given by

$$L(w; \mathcal{D}) = ??$$
.

Note that the distribution on X is here not relevant.

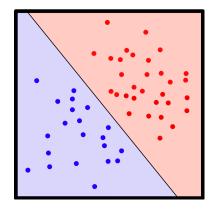
MLE for the logistic regression

• Maximizing L is equivalent to minimizing the negative log-likelihood which gives rise to the error function:

$$E(w) = -\sum_{i=1}^{N} \{y_i \log(\sigma_i(w)) + (1 - y_i) \log(1 - \sigma_i(w))\}, \quad \sigma_i = \sigma(w^{\mathrm{T}} x_i).$$

- E is the called the cross-entropy error function.
- The gradient of E is given by
- The problem of minimizing E does not admit explicit solutions.
- We must use optimization algorithms such as GD or SGD.

Overfitting phenomenon for the logistic regression



• In the case the data is linearly separable: i.e., there exists $\bar{w} \in \mathbb{R}^d$ such that

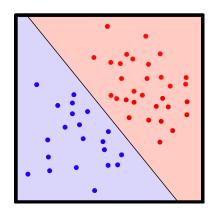
$$\{x_i : y_i = 1\} \subset \mathsf{H}_- = \{x : \bar{w}^{\mathrm{T}} x < 0\},\$$

 $\{x_i : y_i = 0\} \subset \mathsf{H}_+ = \{x : \bar{w}^{\mathrm{T}} x > 0\}.$

then MLE for logistic regression exhibits severe overfitting.

- MLE tends to provide parameters $\hat{w} = \alpha \bar{w}, \ \alpha \in \mathbb{R}$, with $|\alpha|$ very large.
- This results in predictive $p_{\hat{w}}(1|x_{\text{new}})$ which tends to the non-smooth Heaviside function: $\mathbb{1}\left\{\bar{w}^{\text{T}}x<0\right\}$.
- Problem remains even as N is large.

Overfitting phenomenon for the logistic regression



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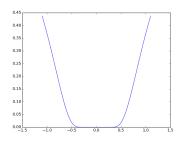
$$\{x_i : y_i = 1\} \subset \mathsf{H}_- = \{x : \bar{w}^\mathrm{T} x < 0\},\$$

 $\{x_i : y_i = 0\} \subset \mathsf{H}_+ = \{x : \bar{w}^\mathrm{T} x > 0\}.$

then MLE for logistic regression exhibits severe overfitting.

- Reason: in that situation, the MLE is not unique and there exists an infinite numbers of solutions
- Standard MLE procedure does not provide a way to favor one solution over another.
- Solution: take a prior on w and consider the MAP instead of the MLE.

Vanishing gradient for the logistic regression



- GD for logistic regression can be slow since E exhibits flat regions;
- this implies vanishing gradients...
- To better understand this phenomenon and accelerate the convergence, we make use of the Hessian of E:

$$\nabla_w^2 E(w) = \left(\frac{\partial^2 E}{\partial w_i w_j}(w)\right)_{i,j=1}^d$$

Convexity of the logistic regression and vanishing gradient phenomenon

• From the expression for $\nabla^2 E$, we can show that E is convex

Proof.

- However, $\min \operatorname{Spec} \nabla^2 E(w) \approx 0$ and also $\nabla E(w) \approx 0$ near minimums. This mathematically formalizes the previous statements.
- Therefore, while E is convex, the convergence will be very slow.
- To get faster convergence, we need to take into account this observation.
- Example 🔌 .

Iterated reweighted least square/ Newton algorithm

- Newton algorithm aims to deal with the problem of vanishing gradient.
- It acts as an adaptive pre-conditioned gradient descent scheme.
- Pre-conditioned gradient descent scheme?

Iterated reweighted least square/ Newton algorithm

- Newton algorithm aims to deal with the problem of vanishing gradient.
- It acts as an adaptive pre-conditioned gradient descent scheme.
- It defines the recursion:

$$w_{k+1} = w_k - \{\nabla^2 E(w_k)\}^{-1} \nabla E(w_k)$$
.

• Example 🔌 .

Multiclass logistic regression

- ullet We aim to generalize the logistic regression for Y = $\{1,\ldots K\},\ K>2.$
- Recall that we start with the statistical model:

$$Y \sim \text{Ber}(\sigma(w,X))$$
,

where σ is an activation function.

• This generalizes easily as

$$Y \sim \text{Multi}(\sigma_1(W, X), \dots, \sigma_K(W, X)), \quad W = [w_1 \cdots w_K] \in \mathbb{R}^{d \times K},$$

where

$$\sigma: \mathbb{R}^{d \times K} \times \mathsf{X} \to \mathrm{Simplex}_K = \{(\varpi_1, \dots, \varpi_K) \in [0, 1]^K : \sum_{k=1}^K \varpi_k = 1\}.$$

 This comes from our previous discussion on generative probabilistic models.

Multiclass logistic regression

- We consider the multiclass setting using logistic regression.
- The logistic model generalizes easily as

$$Y \sim \mathsf{Multi}(\sigma_1(W, X), \dots, \sigma_K(W, X)) , \quad W = [w_1 \cdots w_K] \in \mathbb{R}^{d \times K} ,$$

where

$$\boldsymbol{\sigma}: \mathbb{R}^{d \times K} \times \mathsf{X} \to \operatorname{Simplex}_{K} = \{(\varpi_{1}, \dots, \varpi_{K}) \in [0, 1]^{K} \ : \ \textstyle \sum_{k=1}^{K} \varpi_{k} = 1\},$$

$$\sigma_k(W,X) = \operatorname{softmax}(X^{\mathrm{T}}w_1,\ldots,X^{\mathrm{T}}w_K)_k = \frac{\exp(X^{\mathrm{T}}w_k)}{\sum_{j'=1}^K \exp(X^{\mathrm{T}}w_{j'})}.$$

- This comes from our previous discussion on generative probabilistic models again...
- The likelihood is then given by (we skip as usual the prior on X)

$$L(W; D) = \prod_{i=1}^{N} \mathbb{P}(Y_i = y_i | X = x_i) = \prod_{i=1}^{N} \prod_{k=1}^{K} \{\sigma_{k,i}\}^{y_i = k},$$

setting

$$\sigma_{k,i} = \boldsymbol{\sigma}_k(\boldsymbol{W}, x_i)$$
.

Multiclass logistic regression

• The likelihood is then given by (we skip as usual the prior on X)

$$L(W; D) = \prod_{i=1}^{N} \mathbb{P}(Y_i = y_i | X = x_i) = \prod_{i=1}^{N} \prod_{k=1}^{K} \{\sigma_{k,i}\}^{y_i = k},$$

setting

$$\sigma_{k,i} = \sigma_k(W,x_i)$$
.

• Using the 1-of-K coding for the labels, $t_{k,i} = 1$ $\{y_i = k\}$ and taking the logarithm, we get

$$E(\mathbf{W}) = -\log L(\mathbf{W}; \mathcal{D}) = -\sum_{i=1}^{N} \sum_{k=1}^{K} t_{k,i} \log(\sigma_{k,i}).$$

- $P_{\nabla_W E}$.

Probit regression

 We focus on a {0,1} classification task and consider a discriminative probabilistic model:

$$Y \sim \operatorname{Ber}(\sigma(w^{\mathrm{T}}X))$$
,

where $\sigma: \mathbb{R} \to [0,1]$ is an activation function.

- For the logistic regression, we simply take the logistic sigmoid function.
- ullet However, we can take any cumulative distribution function on \mathbb{R} , F, for $\sigma...$
- The probit regression just consists in taking $\sigma = \Phi$ where Φ is the cumulative distribution function associated with N(0,1):

$$\Phi(t) = \int_{-\infty}^{t} e^{-u^2/2} du/(2\pi)^{1/2}$$
.

- Exercise: write the likelihood associated with the probit regression model for $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$.
- Then w is inferred as the logistic regression by maximum likelihood estimation.
- Again the maximum of the likelihood does not admit a close form and gradient descent, SGD or Newton algorithm has to be used...

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Bayesian logistic regression

Posterior distribution

- Recall that the likelihood associated with the logistic regression model for $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ is?
- Taking a prior for w, p_{prior}, we get using the Bayes formula with the posterior distribution

$$p(w|\mathcal{D}) \propto L(w; \mathcal{D}) \times p_{prior}(w)$$
.

 Following the same discussion as the Bayesian linear regression, Bayesian classification is based on the posterior predictive distribution defined by

$$p(y_{\text{pred}}|x_{\text{new}}) = \int ??.$$

- This integral is not tractable! because the posterior distribution cannot be sampled from.
- In the sequel, we present an approximation method of the posterior.

Laplace approximation method

ullet Here we consider a general target posterior distribution on \mathbb{R}^d

$$p(w|\mathcal{D}) = \lambda(w)/Z$$
, $\lambda(w) = L(w; \mathcal{D})p_{\mathsf{prior}}(w)$, $Z = \int \lambda(w)dw$.

- Here the density is known up to a multiplicative constant: λ is known but not Z.
- ullet The basic idea of Laplace approximation is to find μ and $\Sigma\succeq 0$ such that

$$p(\cdot|\mathcal{D}) \approx N(\mu, \Sigma)$$
.

- Theoretical justification: Berstein von Mises theorem shows that an appropriate scaled version of the posterior converges to a Gaussian distribution.
- $oldsymbol{?}_{\mathsf{which}\;\mu,oldsymbol{\Sigma}}$
- ullet We consider for μ the MAP estimator:

$$w_{\text{MAP}} = \operatorname{argmax} p(\cdot|\mathcal{D}) = \operatorname{argmax} \lambda$$
.

- Basic idea: $p(\cdot|\mathcal{D})$ concentrates around w_{MAP} .
- Remains the choice of Σ .

Laplace approximation method

ullet Here we consider a general target posterior distribution on \mathbb{R}^d

$$p(w|\mathcal{D}) = e^{-E(w)}/Z$$
, $e^{-E(w)} = L(w; \mathcal{D})p_{\mathsf{prior}}(w)$, $Z = \int \lambda(w)\mathrm{d}w$.

ullet The basic idea of Laplace approximation is to find μ and $\Sigma\succeq$ such that

$$p(\cdot|\mathcal{D}) \approx N(\mu, \Sigma)$$
.

ullet We consider for μ the MAP estimator:

$$w_{\text{MAP}} = \operatorname{argmax} p(\cdot|\mathcal{D}) = \operatorname{argmin} E$$
.

ullet For Σ , consider first d=1 and making a second Taylor expansion at $w_{
m MAP},$ we get

$$\begin{split} \log p(w|\mathcal{D}) &\approx \log p(w_{\text{MAP}}|\mathcal{D}) + [\partial_w \log p(w_{\text{MAP}}|\mathcal{D})](w - w_{\text{MAP}}) \\ &+ (1/2)[\partial_w^2 \log p(w_{\text{MAP}}|\mathcal{D})](w - w_{\text{MAP}})^2 \\ &\approx \log p(w_{\text{MAP}}|\mathcal{D}) - (1/2)E''(w_{\text{MAP}})(w - w_{\text{MAP}})^2 \;. \end{split}$$

• This suggests to take

$$\Sigma = 1/E''(w_{\mathrm{MAP}}) \;, \; \mathrm{if} \; E''(w_{\mathrm{MAP}})
eq 0 \;.$$

Laplace approximation method

ullet Here we consider a general target posterior distribution on \mathbb{R}^d

$$p(w|\mathcal{D}) = e^{-E(w)}/Z$$
, $e^{-E(w)} = L(w; \mathcal{D})p_{prior}(w)$, $Z = \int e^{-E(w)}dw$.

• The basic idea of Laplace approximation is to find μ and $\Sigma \succeq$ such that

$$p(\cdot|\mathcal{D}) \approx N(\mu, \Sigma)$$
.

• We consider for μ the MAP estimator:

$$w_{\text{MAP}} = \operatorname{argmax} p(\cdot|\mathcal{D}) = \operatorname{argmin} E$$
.

ullet The previous derivation generalizes for d>1 and we obtain

$$\Sigma = \left[\nabla^2 E(w_{\text{MAP}})\right]^{-1}.$$

• Note that we do not need Z to compute $w_{\rm MAP}$ and Σ since they can only be related to E.

Application to the Bayesian Logistic regression

• Recall that the posterior has a form

$$-\log p(w|\mathcal{D}) = E + \mathrm{Cst} \; ,$$

$$E = \frac{1}{2}(w - m_0) \boldsymbol{S}_0^{-1}(w - m_0) - \sum_{i=1}^N \{y_i \log(\sigma_i) + (1 - y_i) \log(1 - \sigma_i)\}$$

where

$$\sigma_i = ??$$

• Assume that we have estimated the MAP, w_{MAP} , the Hessian for E is

$$\nabla^2 E(w_{\text{MAP}}) = ??$$

• Finally the Laplace approximation is

$$p_{\text{laplace}}(w|\mathcal{D}) = N(w_{\text{MAP}}, [\nabla^2 E(w_{\text{MAP}})]^{-1})$$

Predictive distribution

• The Laplace approximation is

$$p_{\mathrm{laplace}}(w|\mathcal{D}) = \mathsf{N}(w_{\mathrm{MAP}}, \left[\nabla^2 E(w_{\mathrm{MAP}})\right]^{-1})$$

• The predictive distribution is itself approximated by

$$\begin{split} p_{\mathsf{pred}}(y|x_{\mathsf{new}}) &= \int p_w(y|x) p(w|\mathcal{D}) \mathrm{d}w \approx \int p_w(y|x) p_{\mathsf{laplace}}(w|\mathcal{D}) \mathrm{d}w \\ &= \mathbb{E} \left[\sigma(W^{\mathsf{T}} x_{\mathsf{new}}) \right] \;, \qquad W \sim \mathsf{N}(w_{\mathsf{MAP}}, [\nabla^2 E(w_{\mathsf{MAP}})]^{-1}) \\ &= \mathbb{E} \left[\sigma(G(x_{\mathsf{new}})) \right] \;, \qquad G(x_{\mathsf{new}}) \sim ?? \end{split}$$

• $\mathbb{E}\left[\sigma(G(x_{\mathsf{new}}))\right]$ has to be approximated, cannot be evaluated analytically.

Application to the Bayesian Probit regression

• Recall that the posterior has a form

$$-\log p(w|\mathcal{D}) = E + Cst ,$$

$$E = \dots ,$$

• Assume that we have estimated the MAP, w_{MAP} , the Hessian for E is

$$\nabla^2 E(w_{\text{MAP}}) = ??$$

• Finally the Laplace approximation is

$$p_{\text{laplace}}(w|\mathcal{D}) = N(w_{\text{MAP}}, [\nabla^2 E(w_{\text{MAP}})]^{-1}).$$

Predictive distribution

• The Laplace approximation is

$$p_{\mathrm{laplace}}(w|\mathcal{D}) = \mathsf{N}(w_{\mathrm{MAP}}, \left[\nabla^2 E(w_{\mathrm{MAP}})\right]^{-1})$$

• The predictive distribution is itself approximated by

$$\begin{split} p_{\mathsf{pred}}(y|x_{\mathsf{new}}) &= \int p_w(y|x) p(w|\mathcal{D}) \mathrm{d}w \approx \int p_w(y|x) p_{\mathsf{laplace}}(w|\mathcal{D}) \mathrm{d}w \\ &= \mathbb{E} \left[\Phi(W^{\mathsf{T}} x_{\mathsf{new}}) \right] \;, \qquad W \sim \mathsf{N}(w_{\mathsf{MAP}}, [\nabla^2 E(w_{\mathsf{MAP}})]^{-1}) \\ &= \mathbb{E} \left[\Phi(G(x_{\mathsf{new}})) \right] \;, \qquad G(x_{\mathsf{new}}) \sim ?? \end{split}$$

Model comparison and BIC

 For model comparison, recall that we aim to compute the normalizing constant/marginal likelihood

$$\mathrm{e}^{-E(w)} = \mathrm{L}(w; \mathcal{D}) p_{\mathsf{prior}}(w) \;, \quad \mathrm{Z}(\mathcal{M}) = \int \mathrm{e}^{-E(w)} \mathrm{d}w \;.$$

- Here we drop the dependency with respect to $\mathcal M$ which specifies p_{prior} or hyperparameters.
- The larger $Z(\mathcal{M})$ is, the better \mathcal{M} is.
- We can apply the same approximation procedure directly to E(w):

$$E(w) \approx E(w_{\text{MAP}}) + \nabla E(w_{\text{MAP}})(w - w_{\text{MAP}}) + (1/2)\nabla^2 E(w_{\text{MAP}})(w - w_{\text{MAP}})$$
.

• This gives then that

$$\begin{split} \log \mathrm{Z} &\approx -E(w_{\mathrm{MAP}}) - (1/2) \log \det(\nabla^2 E(w_{\mathrm{MAP}})) + (d/2) \log(2\pi) \\ &\approx \log \mathrm{L}(w_{\mathrm{MAP}}; \mathcal{D}) + \log p_{\mathrm{prior}}(w_{\mathrm{MAP}}) \\ &\qquad - (1/2) \log \det(\nabla^2 E(w_{\mathrm{MAP}})) + (d/2) \log(2\pi) \;. \end{split}$$

Model comparison and BIC

 For model comparison, recall that we aim to compute the normalizing constant/marginal likelihood

$$\mathrm{e}^{-E(w)} = \mathrm{L}(w;\mathcal{D}) p_{\mathsf{prior}}(w) \;, \quad \mathrm{Z}(\mathcal{M}) = \int \mathrm{e}^{-E(w)} \mathrm{d}w \;.$$

• The Laplace approximation is

$$\log Z \approx \log L(w_{\text{MAP}}; \mathcal{D}) + \log p_{\text{prior}}(w_{\text{MAP}})$$

$$- (1/2) \log \det(\nabla^2 E(w_{\text{MAP}})) + (d/2) \log(2\pi) .$$
(1)

• Approximating $\log \det(\nabla^2 E(w_{\text{MAP}})) \approx d \log(N)$ gives rise to the Bayesian Information Criterion (BIC) or the Schwarz criterion:

$$\mathrm{BIC} = \log L(w_{\mathrm{MAP}}; \mathcal{D}) - (d/2) \log(N) .$$

- BIC can also give misleading results.
- In particular, the assumption that the Hessian matrix has full rank is often not valid since many of the parameters are not "well-determined".
- As possible, use (1)!

Further reading

- Relation between Fisher linear discriminant and least-square estimation [Bis07, Section 4.1.5];
- 4.3.6 Canonical link functions

Bibliography i

[Bis07] Christopher M. Bishop. Pattern Recognition and Machine Learning (Information Science and Statistics). 1st ed. Springer, 2007. ISBN: 0387310738.