Probabilistic Models

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Machine Learning

Outline

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Predictions based on Probability

- Supervised learning, we are given a training set $\mathbb{X} = \{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}_{i=1}^{N}$

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- *Maximum likelihood (ML) estimation*:

$$\arg\max_{\Theta} \mathrm{P}(\mathbb{X} \,|\, \Theta)$$

  - Assumes uniform $\mathrm{P}(\Theta)$ and does not prefer particular Θ

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- ML estimation:

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- The optimal point does not change since $\log$ is monotone increasing

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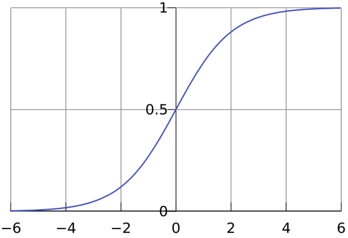
- How to relate $\boldsymbol{x}$ to ρ?

Logistic Function

- Recall that the ***logistic function***

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

is commonly used as a parametrizing function of the Bernoulli distribution



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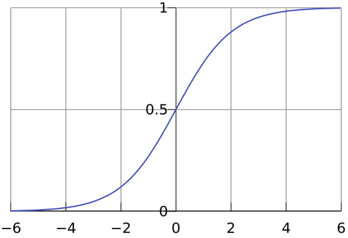

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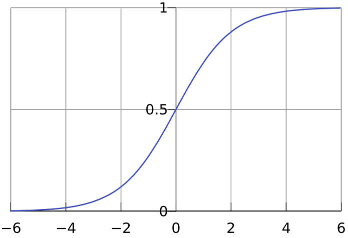

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$= \arg\max_{y} \{(A), (B)\}$

- How to learn $\boldsymbol{w}$ from $\mathbb{X}$?

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- In *logistic regression*, we let

$$z = \boldsymbol{w}^\top \boldsymbol{x}$$

  - Basically, z is the projection of $\boldsymbol{x}$ along the direction $\boldsymbol{w}$
- We have

$$\mathrm{P}(y \mid \boldsymbol{x}; \boldsymbol{w}) = \sigma(\boldsymbol{w}^\top \boldsymbol{x})^{y'} [1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x})]^{(1-y')}$$

- Prediction:

$$\hat{y} = \arg\max_{y} \mathrm{P}(y \mid \boldsymbol{x}; \boldsymbol{w}) = \mathrm{sign}(\boldsymbol{w}^\top \boldsymbol{x})$$

- How to learn $\boldsymbol{w}$ from $\mathbb{X}$?
- ML estimation:

$$\arg\max_{\boldsymbol{w}} \mathrm{P}(\mathbb{X} \mid \boldsymbol{w})$$

ML Estimation

- Log-likelihood:

$$
\begin{aligned}
\log \mathrm{P}(\mathbb{X} \,|\, \boldsymbol{w}) &= \log \prod_{i=1}^{N} \mathrm{P}\left(\boldsymbol{x}^{(i)}, y^{(i)} \,|\, \boldsymbol{w}\right) \\
&= \log \prod_{i} \mathrm{P}\left(y^{(i)} \,|\, \boldsymbol{x}^{(i)}, \boldsymbol{w}\right) \mathrm{P}\left(\boldsymbol{x}^{(i)} \,|\, \boldsymbol{w}\right)
\end{aligned}
$$

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- Unlike in linear regression, we cannot solve $\boldsymbol{w}$ analytically in a closed form via

$$\nabla_{\boldsymbol{w}} \log \mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w}) = \sum_{t=1}^{N} [y'^{(i)} - \sigma(\boldsymbol{w}^\top \boldsymbol{x}^{(i)})]\boldsymbol{x}^{(i)} = \mathbf{0}$$

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不好解

- However, we can still evaluate $\nabla_{\boldsymbol{w}} \log \mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w})$ and use the iterative methods to solve $\boldsymbol{w}$
  - E.g., stochastic gradient descent

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- However, we can still evaluate $\nabla_{\boldsymbol{w}} \log \mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w})$ and use the iterative methods to solve $\boldsymbol{w}$
  - E.g., stochastic gradient descent
- It can be shown that $\log \mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w})$ is concave in terms of $\boldsymbol{w}$ [1]
  - So, iterative algorithms converges

Outline

MAP Estimation

- So far, we solve $\boldsymbol{w}$ by ML estimation:

$$\arg\max_{\boldsymbol{w}} \mathrm{P}(\mathbb{X} \,|\, \boldsymbol{w})$$

MAP Estimation

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- In MAP estimation, we solve 較符合直覺 根據一組X 去推測最好的W

$$\arg\max_{\boldsymbol{w}} \mathrm{P}(\boldsymbol{w} \mid \mathbb{X}) = \arg\max_{\boldsymbol{w}} \mathrm{P}(\mathbb{X} \mid \boldsymbol{w}) \mathrm{P}(\boldsymbol{w})$$

- $\mathrm{P}(\boldsymbol{w})$ models our ***preference*** or ***prior knowledge*** about $\boldsymbol{w}$

MAP Estimation for Linear Regression

- MAP estimation in linear regression:

$$\arg\max_{\boldsymbol{w}} \log[\mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w})\mathrm{P}(\boldsymbol{w})]$$

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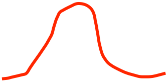

0

$$\log[\mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w})\mathrm{P}(\boldsymbol{w})] = \log \mathrm{P}(\mathbb{X}\,|\,\boldsymbol{w}) + \log \mathrm{P}(\boldsymbol{w})$$

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- $\mathrm{P}(\boldsymbol{w})$ corresponds to the ***weight decay*** term in Ridge regression
- MAP estimation provides a way to design complicated yet interpretable regularization terms
  - E.g., we have LASSO by letting $\mathrm{P}(\boldsymbol{w}) \sim \mathrm{Laplace}(0, b)$ [Proof]
  - We can also let $\mathrm{P}(\boldsymbol{w})$ be a mixture of Gaussians

Remarks on ML and MAP Estimation

Theorem (Consistency)

*The ML estimator Θ_{ML} is **consistent**, i.e., $\lim_{N\to\infty}\Theta_{ML} \xrightarrow{\Pr} \Theta^*$ as long as the "true" $\mathrm{P}(y\,|\,\boldsymbol{x};\Theta^*)$ lies within our model $\mathbb{F}$.*

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Theorem (Cramér-Rao Lower Bound [2])

At a fixed (large) number N of examples, no consistent estimator of Θ^* has a lower expected MSE (mean square error) than the ML estimator Θ_{ML}.

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有著夠大的data set ＭＬ可以learn的最好

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- When N is small that yields overfitting behavior, we can use MAP estimation to ***introduce bias*** and ***reduce variance***

data set太小的話

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Outline

Bayesian Estimation

- In ML/MAP estimation, we solve Θ first, then uses it as a constant to make prediction:

$$\hat{\boldsymbol{y}} = \arg\max_{\boldsymbol{y}} \mathrm{P}(\boldsymbol{y} \,|\, \boldsymbol{x}; \Theta)$$

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- ***Bayesian estimation*** threats Θ as a random variable:

$$\hat{\boldsymbol{y}} = \arg\max_{\boldsymbol{y}} \mathrm{P}(\boldsymbol{y} \,|\, \boldsymbol{x}, \mathbb{X}) = \arg\max_{\boldsymbol{y}} \int \mathrm{P}(\boldsymbol{y}, \Theta \,|\, \boldsymbol{x}, \mathbb{X}) d\Theta$$

  - Makes prediction by considering ***all*** Θ's (weighted by their chances)

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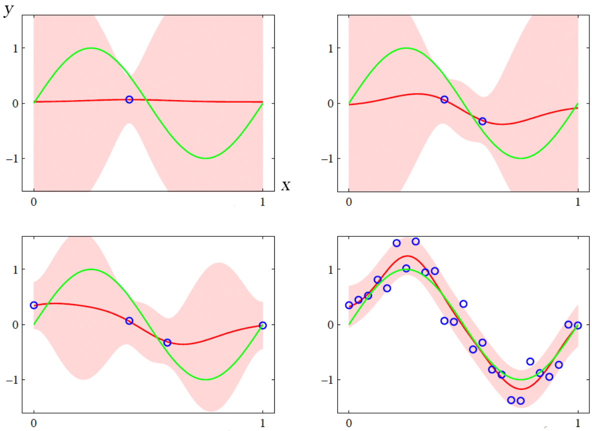
- Bayesian estimation usually generalizes much better when the size N of training set is small

Bayesian vs. ML Estimation

- Example: polynomial regression



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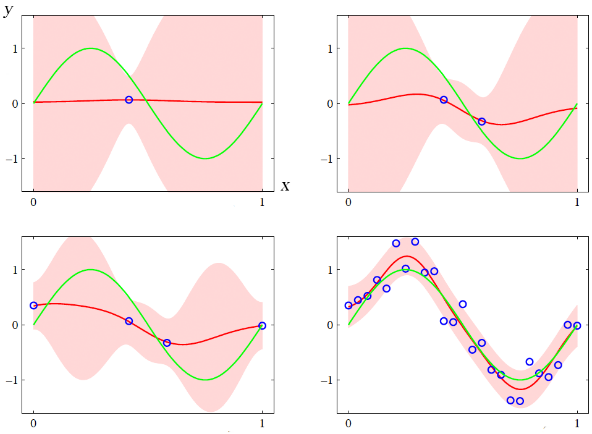

Bayesian vs. ML Estimation

- Example: polynomial regression
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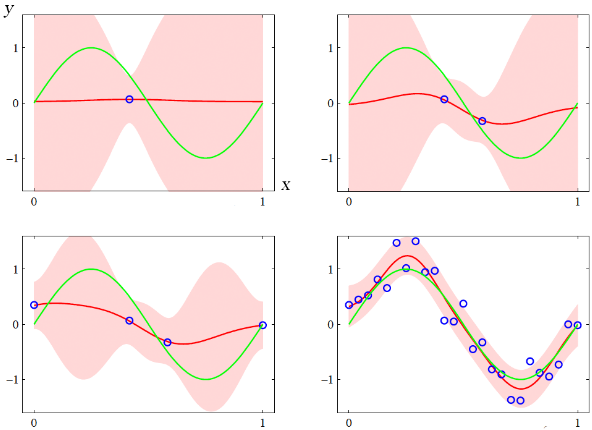
- Shaded area: predictions by ML/MAP estimation regressors



Bayesian vs. MAP Estimation

- MAP gains some benefit of Bayesian approach by incorporating prior as $\mathrm{bias}(\Theta_{\mathsf{MAP}})$
  - Reduces $\mathrm{Var}_{\mathbb{X}}(\Theta_{\mathsf{MAP}})$ when training set is small

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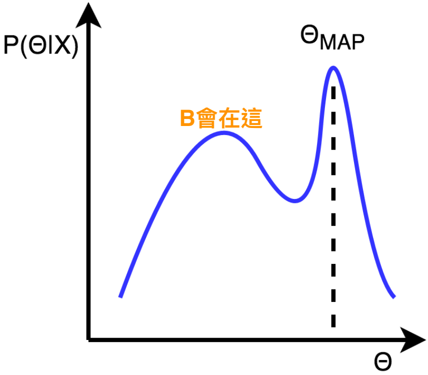
- MAP gains some benefit of Bayesian approach by incorporating prior as $\mathrm{bias}(\Theta_{\mathrm{MAP}})$
  - Reduces $\mathrm{Var}_{\mathbb{X}}(\Theta_{\mathrm{MAP}})$ when training set is small
- However, does ***not*** work if Θ_{MAP} is unrepresentative of the majority Θ in $\int \mathrm{P}(\boldsymbol{y}, \Theta \,|\, \boldsymbol{x}, \mathbb{X}) d\Theta$
- E.g. when $\mathrm{P}(\Theta \,|\, \mathbb{X})$ is a mixture of Gaussian



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- Usually generalizes much better given a small training set
- Unfortunately, solution may not be tractable in many applications
- Even tractable, incurs high computation cost
  - Not suitable for large-scale learning tasks

再夠大的data set下 效果可能比ML/MAP好一點點
但computation cost會高很多

Reference I

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