Machine Learning

Section 10: Model selection & hyper parameter tuning

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(-1).st ~~of~~ ~~10~~ November 2021 ~~2~~

Overview

- Evaluating on test error / cross-validation
- Bayesian model selection
- 根据测试误差/交叉验证进行评估
- 贝叶斯模型选择

Evaluating on test error / cross validation
根据测试误差/交叉验证进行评估

Example: linear regression

Data:

- dataset $\mathcal{D}$ of scalar-valued input/output pairs $(x_1, y_1) \ldots, (x_n, y_n)$
- the outputs are noisy输出是有噪声的

Model:

- basis function $\phi_d(x) = [1, x, x^2, \ldots, x^d]^T$ with hyperparameter d
- model the function as $f(x, w) = \phi_d(x)^T w$, with parameter $w \in \mathbb{R}^{d+1}$

Loss and fit:

- mean-squared error

$$\text{MSE}(\mathcal{D}, w, d) = \frac{1}{|\mathcal{D}|} \sum_{(x,y)\in\mathcal{D}} (y - f(x, w))^2 = \frac{1}{|\mathcal{D}|} \sum_{(x,y)\in\mathcal{D}} (y - \phi_d(x)^T w)^2$$

- minimize the MSE (to get the maximum likelihood estimator):

$$w_{ML}(\mathcal{D}, d) = \arg\min_w \text{MSE}(\mathcal{D}, w, d)$$

Model selection / hyperparameter tuning

- What is the best choice for d?

Hyperparameter tuning: 1st attempt

Idea:

- choose d such that the MSE is minimal:

$$d_1 = \arg\min_d \mathrm{MSE}(\mathcal{D}, w_{ML}(\mathcal{D}, d), d)$$

Problem:

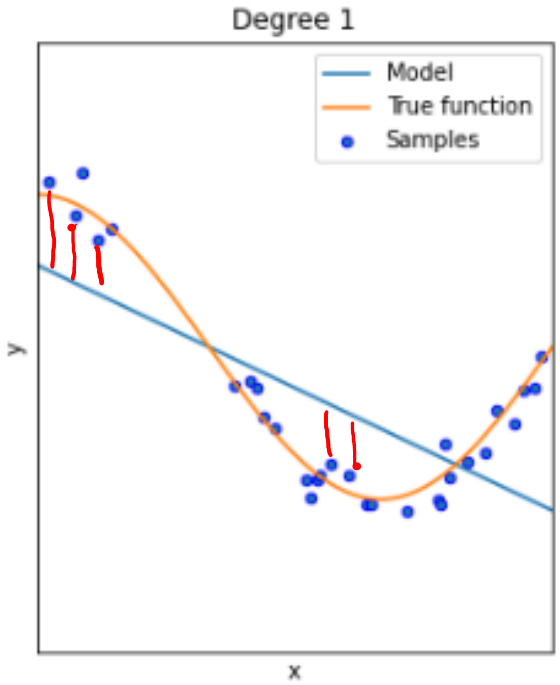
- this overfits the data数据的覆盖
- the best fit will be a large d, such that every single noisy data point is hit最好的拟合将是一个大d，这样每一个嘈杂的数据点都被击中
- however, actually, we would like to minimize the *test error* which is the MSE on unseen data
  然而，实际上，我们希望最小化测试误差，即未见过的数据的MSE
- idea: split data into seen (training) and unseen (evaluation) data
- 思路：将数据分成已见数据（训练）和未见数据（评估）

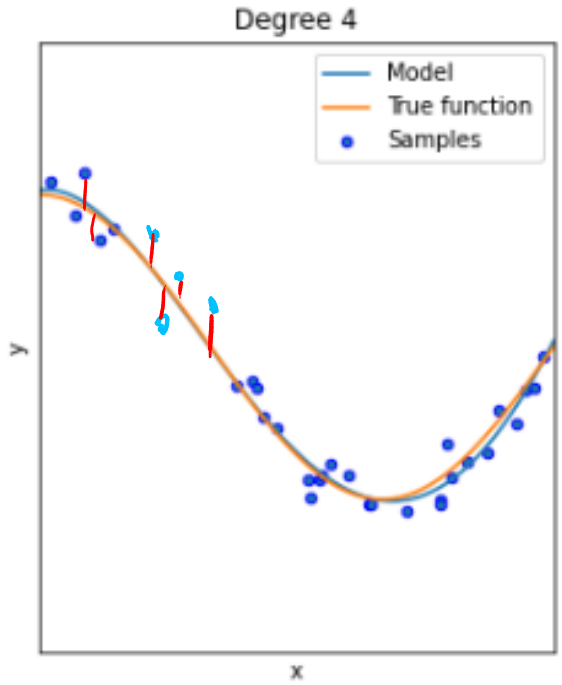
```
def phi(x, d):
    return np.dstack([np.power(x, i) for i in range(d+1)]).squeeze()
```

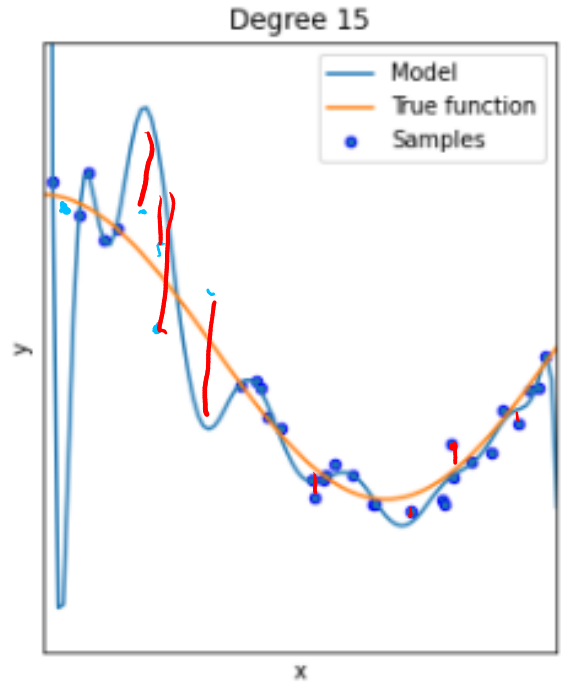
```
def poly_regression_plot(x, y, d):
    # perform regression analysis:
    transformed_x = phi(x, d)

    linear_regressor = LinearRegression()
    linear_regressor.fit(transformed_x, y)
    Y_pred = linear_regressor.predict(transformed_x)
```

Capacity of model →







big MSE

training error: large

underfitting

small MSE

medium

smallest MSE

small

overfitting

Aside: Polynomial regression will always lead MSE = 0 for high enough degree

$$\underbrace{\begin{pmatrix} x_1^d & x_1^{d-1} & \dots & x_1 & 1 \\ & & & & \\ & & & & \\ x_{d+1}^d & x^{d-1} & \dots & x_{d+1} & 1 \end{pmatrix}}_{=:A} \begin{pmatrix} w_1 \\ \vdots \\ w_{d+1} \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_{d+1} \end{pmatrix}$$

$$\det(A) = \prod_{i<j} (x_i - x_j) \neq 0$$ if all x_i different

$\rightsquigarrow$ always solvable ...

Hyperparameter tuning: 2nd attempt超参数调整

Idea:

- split dataset $\mathcal{D}$ into two disjoint sets $\mathcal{D}_{\text{train}}$ and $\mathcal{D}_{\text{eval}}$
- 1. *train* on $\mathcal{D}_{\text{train}}$ (choose parameter w)
  2. *evaluate* on $\mathcal{D}_{\text{eval}}$ (choose hyperparameter d)
- choose d such that the MSE on the evaluation set is minimal for the parameter w chosen on the training set:

$$d_2 = \arg\min_d \text{MSE}(\mathcal{D}_{\text{eval}}, w_{ML}(\mathcal{D}_{\text{train}}, d), d)$$

Note:

- much better! works quite well!
- no overfitting while learning the parameter

Problems/challenges:

- how good is the parameter/hyperparameter choice on unseen data? i.e. what is the *test error* (the MSE on unseen data)?
- the estimator $\text{MSE}(\mathcal{D}_{\text{eval}}, w_{ML}(\mathcal{D}_{\text{train}}, d_2), d_2)$ of the MSE is too optimistic (this is similar to underestimating the variance with a sample mean)

Typical evaluation diagram:

$$\arg\min_d \; MSE(D_{test}, d)$$

Data splitting:

```python
from sklearn.model_selection import train_test_split

X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.2)
```

Grid search:

for i in range(500):

$X\_train = [1, X, X^2, \ldots, X^i]$

linear_model.fit(X_train, Y_train)

$MSE[i] = \frac{1}{|X\_test|} (linear\_model.predict(X\_test) - Y\_test)^2$ .sum()

Pick $d = \underset{i}{\text{argmin}}\ MSE[i]$

Can have several hyperparameters:

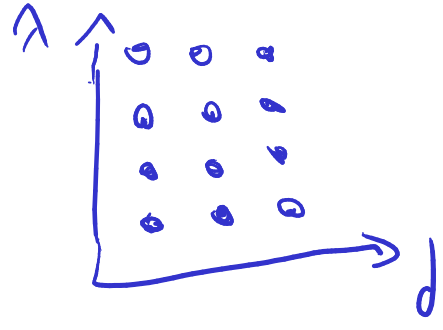
E.g. degree d

$$
\begin{aligned}
w_{\text{ridge}} &= \text{argmax}_w \, p(w|X,y) = \text{argmax}_w \, p(y|X,w)p(w|X)/p(y|X) \\
&= \text{argmax}_w \, p(y|X,w)p(w) \\
&= \text{argmax}_w \sum_{i=1}^{n} \log \mathcal{N}(y_i|x_i^T w, \sigma^2) + \sum_{j=1}^{d} \log \mathcal{N}(w_j|0,\tau^2) \\
&= \text{argmin}_w \underbrace{\frac{1}{n}\sum_{i=1}^{n}(y_i - x_i^T w)^2}_{\text{fit}} + \underbrace{\lambda \|w\|_2^2}_{\text{regularizer}}
\end{aligned}
$$

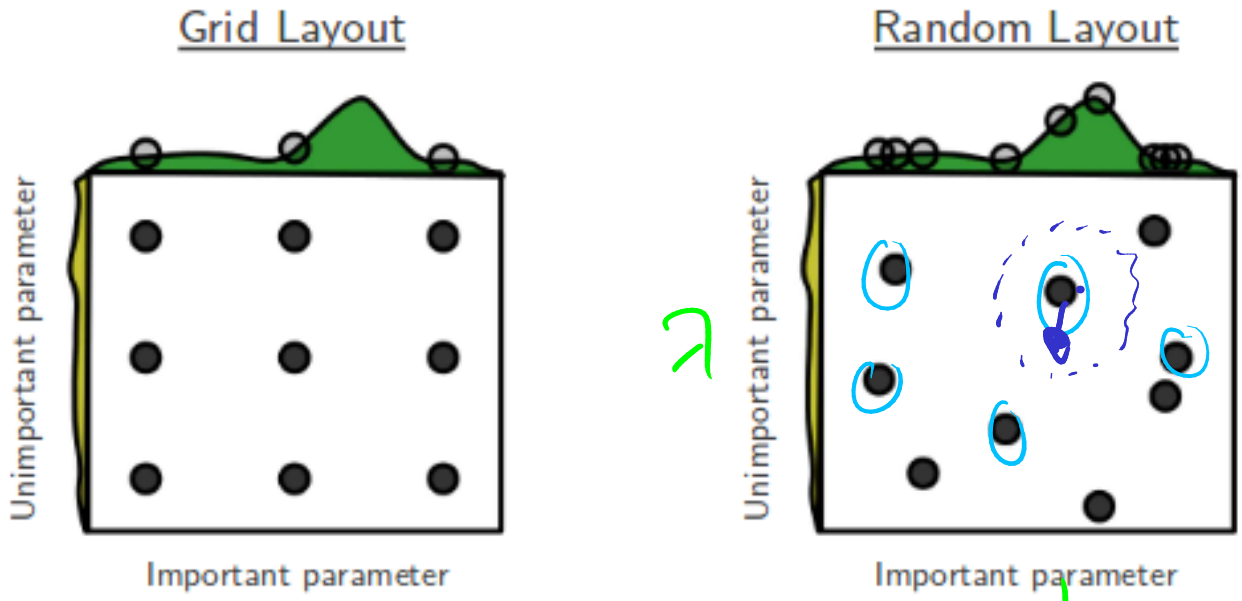
RIDGE REGR.

... and regularization constant λ

⇝ Grid search



Grid search vs. random search:



(Stolen by Bengio 2012)

Alternative for continuous hyperparams λ:

- Write function for test error
- do „automatic differentiation"
- follow the gradient to lower error

Hyperparameter tuning: 3rd attempt

Idea:

- split dataset $\mathcal{D}$ into three disjoint sets $\mathcal{D}_{\text{train}}$, $\mathcal{D}_{\text{eval}}$ and $\mathcal{D}_{\text{test}}$
- 1. *train* on $\mathcal{D}_{\text{train}}$ (choose parameter w)
  2. *evaluate* on $\mathcal{D}_{\text{eval}}$ (choose hyperparameter d)
  3. *test* of $\mathcal{D}_{\text{test}}$ (calculate MSE for unseen data)

validation data

← e.g. different models.

- choose d such that the MSE on the evaluation set is minimal for the parameter w chosen on the training set:

$$d_3 = \arg\min_d \text{MSE}(\mathcal{D}_{\text{eval}}, w_{ML}(\mathcal{D}_{\text{train}}, d), d)$$

- calculate the test error (the MSE on unseen data) on the test set:

$$\text{MSE}(\mathcal{D}_{\text{test}}, w_{ML}(\mathcal{D}_{\text{train}}, d_3), d_3)$$

Note:

- this is the gold standard (if we have enough data)!
- no overfitting of the parameter or of the hyperparameter

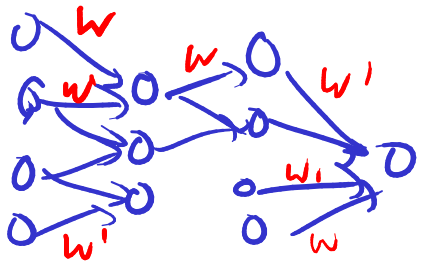
Why the final test?

- estimate success of modelling
- model selection

E.g. Could have:

- polynomial regression
- trigonometric regression
- neural network

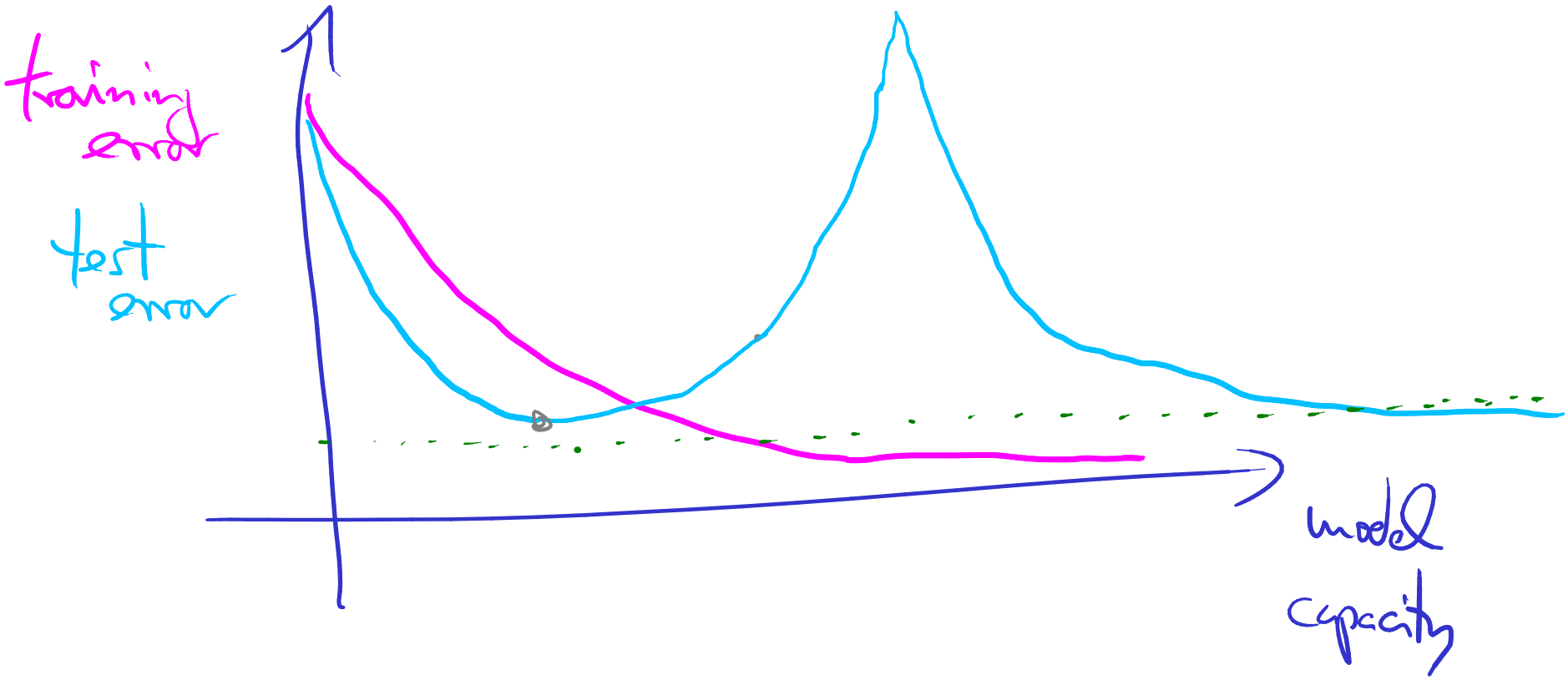
$$\sum_{n=1}^{k} w_n \sin(n \cdot \pi \cdot x)$$



If training (i.e. optimizing w) is costly: (e.g. neural networks)

„epochs"	Grid pts.
1	64
16	16
32	4
64	1

Double descent



Regularization against overfitting:

$$= \operatorname{argmin}_w \underbrace{\frac{1}{n}\sum_{i=1}^{n}(y_i - x_i^T w)^2}_{\text{fit}} + \underbrace{\lambda \|w\|_2^2}_{\text{regularizer}}$$

$$(\lambda_1, \ldots, \lambda_n) \cdot \begin{pmatrix} |w_0| \\ \vdots \\ |w_n| \end{pmatrix}$$

$$\| \cdot \|_1$$

$$\sum_{i=1}^{n} \lambda_i |w_i|$$

Hyperparameter tuning: 3rd attempt - more thoughts

Idea:

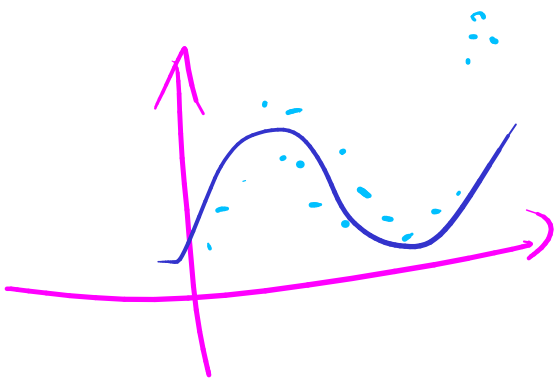
- split dataset $\mathcal{D}$ into three disjoint sets $\mathcal{D}_{\text{train}}$, $\mathcal{D}_{\text{eval}}$ and $\mathcal{D}_{\text{test}}$
- 1. *train* on $\mathcal{D}_{\text{train}}$ (choose parameter *w*)
  2. *evaluate* on $\mathcal{D}_{\text{eval}}$ (choose hyperparameter *d*)
  3. *test* of $\mathcal{D}_{\text{test}}$ (calculate MSE for unseen data)

Problems

- we are not using all data for estimating the parameter
- we are not using all data for estimating the hyperparameter

Hack/Solution

- Cross-validation (see next slide)
- does improve the estimate



Cross-validation (2-fold)

Simpler setup w/o hyperparameter

- given data $\mathcal{D}$
- model with parameter w
- but no hyperparameter d

Goal

- estimate the test error

Solution

- split $\mathcal{D}$ into two sets $\mathcal{D}_1$ and $\mathcal{D}_2$
  1. train w_1 on $\mathcal{D}_1$, estimate MSE ε_1 on $\mathcal{D}_2$ for w_1
  2. train w_2 on $\mathcal{D}_2$, estimate MSE ε_2 on $\mathcal{D}_1$ for w_2
- the cross-validation estimate of the test error is the average:

$$(\varepsilon_1 + \varepsilon_2)/2$$

More general:

Algorithm 10.1 (k-fold cross validation (CV))

Split your data $\mathcal{D}$ into k disjoint subsets of approximately equal size:

$$\mathcal{D} = \mathcal{D}_1 \cup \ldots \cup \mathcal{D}_k$$

For $i = 1$ to k

1. *$\mathcal{D}_i$ plays the role of the test set*
2. *train parameter w on $\mathcal{D} \setminus \mathcal{D}_i$ (i.e. "$\mathcal{D}$ without $\mathcal{D}_i$", set minus)*
3. *calculate MSE ε_i on $\mathcal{D}_i$*

The cross-validation estimate of the test error ε is the average validation error:

$$\varepsilon_{CV} = \frac{1}{k} \sum_{i=1}^{k} \varepsilon_i$$

For $k = n$ this is called leave-one-out cross validation (LOOCV).

$\Rightarrow$ nr. of data points

Nested cross validation for the gold-standard

Setup

- given some data set $\mathcal{D}$
- model with parameter w and hyper-parameter d.

Goal:

- goal: estimate test error目标：估计测试误差

Outer k-fold cross-validation

1. split $\mathcal{D}$ into $\mathcal{D}_1, \ldots, \mathcal{D}_k$
2. for i in $1 \ldots k$:
   - 2.1 split $\mathcal{D}$ into $\mathcal{D} \setminus \mathcal{D}_i$ and $\mathcal{D}_i$
   - 2.2 train w and d on $\mathcal{D} \setminus \mathcal{D}_i$
     use Inner k'-fold cross-validation to estimate the MSE for the hyperparameter choice
   - 2.3 estimate ε_i on $\mathcal{D}_i$ using w and d
3. estimate test error ε as the average of $\varepsilon_1, \ldots, \varepsilon_k$

Bayesian model selection

Bayesian inference

Model specification

$$p(w) = \ldots \qquad \text{prior}$$
$$p(D \mid w) = \ldots \qquad \text{likelihood}$$

Inference given data

$$p(w \mid D) = \frac{p(D \mid w)p(w)}{p(D)} \qquad \text{posterior}$$
$$p(D) = \int p(D \mid w)p(w)dw \qquad \text{evidence}$$

- The *posterior*后验
- *通过乘积法则（贝叶斯法则）将先验和似然结合起来*
  - combines prior and likelihood via product rule (Bayes rule)
  - describes what the parameter might be after seeing data描述看到数据后参数可能是什么
- The *evidence*
  - integrates out the parameter via sum rule
  - is the expected likelihood under the prior通过总和规则整合出参数
  - 证据是先验下的预期可能性

Bayesian inference with hyper-parameters

Model specification

$$p(\theta) = \ldots \qquad \text{hyper-prior (level 2)}$$
$$p(w \mid \theta) = \ldots \qquad \text{prior (level 1)}$$
$$p(D \mid w) = \ldots \qquad \text{likelihood}$$

Level 1: Inference of parameters

$$p(w \mid D, \theta) = \frac{p(D \mid w)p(w \mid \theta)}{p(D \mid \theta)} \qquad \text{posterior}$$
$$p(D \mid \theta) = \int p(D \mid w)p(w \mid \theta)dw \qquad \text{evidence}$$

Level 2: Inference of hyper-parameters

$$p(\theta \mid D) = \frac{p(D \mid \theta)p(\theta)}{p(D)} \qquad \text{hyper-posterior}$$
$$p(D) = \int p(D \mid \theta)p(\theta)d\theta \qquad \text{hyper-evidence}$$

From Murphy, Machine Learning: A probabilistic perspective

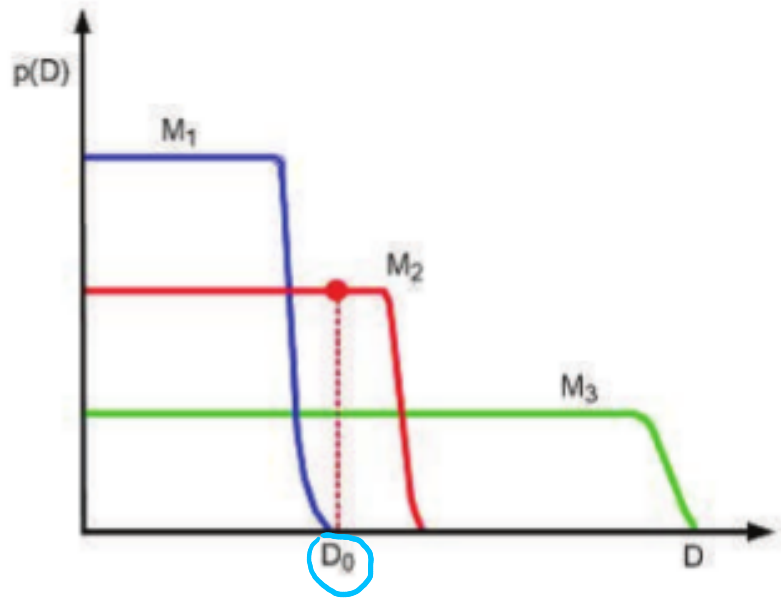


Figure 5.6 A schematic illustration of the Bayesian Occam's razor. The broad (green) curve corresponds to a complex model, the narrow (blue) curve to a simple model, and the middle (red) curve is just right. Based on Figure 3.13 of (Bishop 2006a). See also (Murray and Ghahramani 2005, Figure 2) for a similar plot produced on real data.

McKay: More precise derivation of Occam's razor phenomenon.

Bayesian inference with hyper-parameters and models

Model specification

$$p(\mathcal{H}) = \ldots \quad \text{model-prior (level 3)}$$
$$p(\theta \mid \mathcal{H}) = \ldots \quad \text{hyper-prior (level 2)}$$
$$p(w \mid \theta, \mathcal{H}) = \ldots \quad \text{prior (level 1)}$$
$$p(D \mid w, \mathcal{H}) = \ldots \quad \text{likelihood}$$

Level 1, 2, 3: Inference of parameters, hyper-parameters and model given data

$$p(w \mid D, \theta, \mathcal{H}) = \frac{p(D \mid w, \mathcal{H}) p(w \mid \theta, \mathcal{H})}{p(D \mid \theta, \mathcal{H})} \quad \text{posterior}$$
$$p(\theta \mid D, \mathcal{H}) = \frac{p(D \mid \theta, \mathcal{H}) p(\theta \mid \mathcal{H})}{p(D \mid \mathcal{H})} \quad \text{hyper-posterior}$$
$$p(\mathcal{H} \mid D) = \frac{p(D \mid \mathcal{H}) p(\mathcal{H})}{p(D)} \quad \text{model-posterior}$$

Bayesian inference with hyper-parameters and models

Level 1: Inference of parameters

$$p(w \mid D, \theta, \mathcal{H}) = \frac{p(D \mid w, \mathcal{H}) p(w \mid \theta, \mathcal{H})}{p(D \mid \theta, \mathcal{H})} \quad \text{posterior}$$

$$p(D \mid \theta, \mathcal{H}) = \int p(D \mid w, \mathcal{H}) p(w \mid \theta, \mathcal{H}) dw \quad \text{marginal likelihood}$$

Level 2: Inference of hyper-parameters

$$p(\theta \mid D, \mathcal{H}) = \frac{p(D \mid \theta, \mathcal{H}) p(\theta)}{p(D \mid \mathcal{H})} \quad \text{hyper-posterior}$$

$$p(D \mid \mathcal{H}) = \int p(D \mid \theta, \mathcal{H}) p(\theta \mid \mathcal{H}) d\theta$$

Level 3: Inference of model

$$p(\mathcal{H} \mid D) = \frac{p(D \mid \mathcal{H}) p(\mathcal{H})}{p(D)} \quad \text{model-posterior}$$

$$p(D) = \sum_{\mathcal{H}} p(D \mid \mathcal{H}) p(\mathcal{H})$$

Model selection for regression

Instead of a model for $p(D)$ we specify a model for $p(y \mid X)$ with location matrix X and targets y.

Bayesian model selection for regression

Model specification

$$p(\mathcal{H}) = \ldots \quad \text{model-prior}$$
$$p(\theta \mid \mathcal{H}) = \ldots \quad \text{hyper-prior}$$
$$p(w \mid \theta, \mathcal{H}) = \ldots \quad \text{prior}$$
$$p(y \mid X, w, \mathcal{H}) = \ldots \quad \text{likelihood (this is different)}$$

Level 1, 2, 3: Inference of parameters, hyper-parameters and model given data

$$p(w \mid y, X, \theta, \mathcal{H}) = \frac{p(y \mid X, w, \mathcal{H}) p(w \mid \theta, \mathcal{H})}{p(y \mid X, \theta, \mathcal{H})} \quad \text{posterior}$$
$$p(\theta \mid y, X, \mathcal{H}) = \frac{p(y \mid X, \theta, \mathcal{H}) p(\theta \mid \mathcal{H})}{p(y \mid X, \mathcal{H})} \quad \text{hyper-posterior}$$
$$p(\mathcal{H} \mid y, X) = \frac{p(y \mid X, \mathcal{H}) p(\mathcal{H})}{p(y \mid X)} \quad \text{model-posterior}$$

Bayesian model selection for Linear Regression

Level 1:

$$w \sim \mathcal{N}(0_d, \tau^2 I_d)$$
$$y \mid X, w \sim \mathcal{N}(Xw, \sigma^2 I_n)$$

We infer posterior:

$$w \mid X, y \sim \mathcal{N}(w_n, V_n) \qquad \text{posterior}$$

with posterior mean w_n and posterior covariance V_n.

$$V_n = \left(\frac{1}{\sigma^2} X^T X + \frac{1}{\tau^2} I_d \right)^{-1}$$
$$w_n = (X^T X + \frac{\sigma^2}{\tau^2} I_d)^{-1} X^T y$$

Note that on this slide σ^2 and τ^2 is assumed to be known (constant).

Level 2: Let's add random variables for the hyper-parameters!

Bayesian model selection for Linear Regression

Level 1:

$$\theta \sim \ldots \qquad \text{hyper-prior}$$
$$w \mid \theta \sim \mathcal{N}(0_d, \tau^2 I_d) \qquad \text{prior}$$
$$y \mid X, w, \theta \sim \mathcal{N}(Xw, \sigma^2 I_n) \qquad \text{likelihood}$$

where $\theta = (\sigma^2, \tau^2, d)$ collects all hyperparameter.
We infer posterior:

$$w \mid X, y, \theta \sim \mathcal{N}(w_n, V_n \mid \theta) \qquad \text{posterior}$$

with posterior mean w_n and posterior covariance V_n which do dependent on θ.
Level 2: We need the evidence from level 1:

$$p(y \mid X, \theta) = \int p(y \mid X, w, \theta) p(w \mid \theta) dw = \mathcal{N}(\ldots)$$

This is also called *marginal likelihood*.

Bayesian inference for level 2

Level 2: Infer hyper-posterior:

$$p(\theta \mid y, X) = \frac{p(y \mid X, \theta) p(\theta)}{p(y \mid X)}$$

This gets quickly too complicated! (the integral become to difficult)

Instead we only maximize the Marginal likelihood

$$p(y \mid X, \theta) = \int p(y \mid X, w, \theta) p(w \mid \theta) dw = \mathcal{N}(\ldots)$$

with respect to the hyper-parameter θ.

- this is called “Type II maximum likelihood” and “empirical Bayes” and “generalized maximum likelihood” and “evidence approximation”

Marginal likelihood for linear regression

We can derive the form of the logarithm of the marginal likelihood:

$$
\begin{aligned}
\log p(y \mid X, \theta) &= \log \int p(y \mid X, w, \theta)\, p(w \mid \theta)\, dw \\
&= \log \int \mathcal{N}(y \mid Xw, \sigma^2 I_n)\, \mathcal{N}(w \mid 0_d, \tau^2 I_d)\, dw \\
&= \log \int \mathcal{N}(y \mid 0_n, \sigma^2 I_n + \tau^2 XX^T)\, \mathcal{N}(w \mid \ldots, \ldots)\, dw \\
&= \log \mathcal{N}(y \mid 0_n, \sigma^2 I_n + \tau^2 XX^T) \int \mathcal{N}(w \mid \ldots, \ldots)\, dw \\
&= \log \mathcal{N}(y \mid 0_n, \sigma^2 I_n + \tau^2 XX^T) \\
&= -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log|\sigma^2 I_n + \tau^2 XX^T| - \frac{1}{2} y^T (\sigma^2 I_n + \tau^2 XX^T)^{-1} y
\end{aligned}
$$

Notes:

- $\mathcal{N}(w \mid \ldots, \ldots)$ does not depend on y.
- The third equality follows from some fancy rule for the Gaussians (see next slide).

Another product formula for Gaussians

copied from Bishop's book Sec. 2.3.3, page 93

Given a marginal Gaussian for x and a conditional Gaussian for y given x,

$$x \sim \mathcal{N}(\mu, \Lambda^{-1})$$
$$y \,|\, x \sim \mathcal{N}(Ax + b, L^{-1})$$

we have the following marignal Guassian for y and conditional Gaussian for x given y:

$$y \sim \mathcal{N}(A\mu + b, L^{-1} + A\Lambda^{-1}A^T)$$
$$x \,|\, y \sim \mathcal{N}(\Sigma(A^T L(y - b) + \Lambda\mu), \Sigma)$$

where $\Sigma = (\Lambda + A^T LA)^{-1}$

End of Section 10

Literature on Bayesian model selection / linear regression:

- Chapter 3.5 in Bishop's book "Pattern Recognition and Machine learning"
- Murphy 5.3
- McKay