Regression: a Probabilistic View

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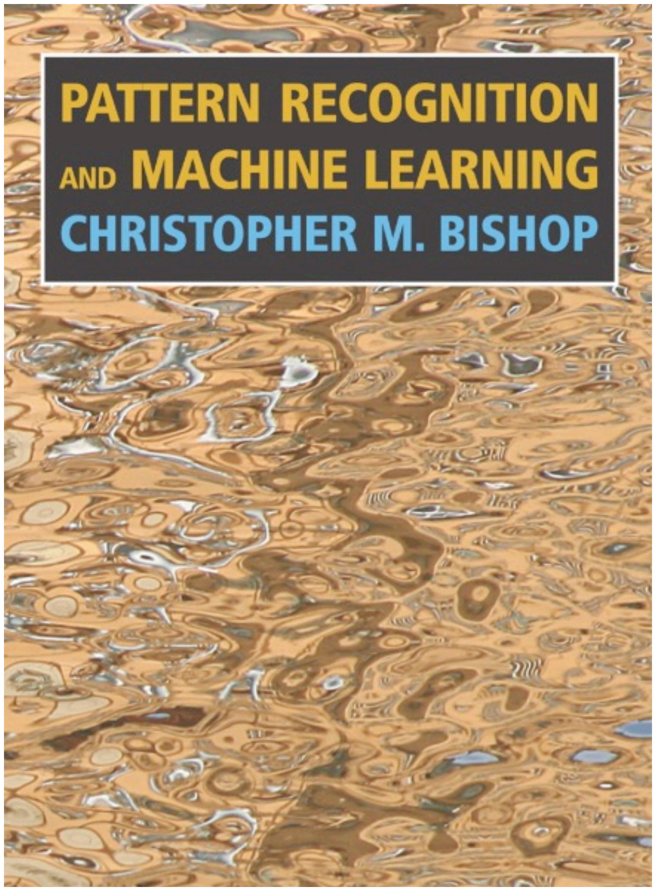
Office Hour: Thursday 3-4pm

Office: GA 18

Reference



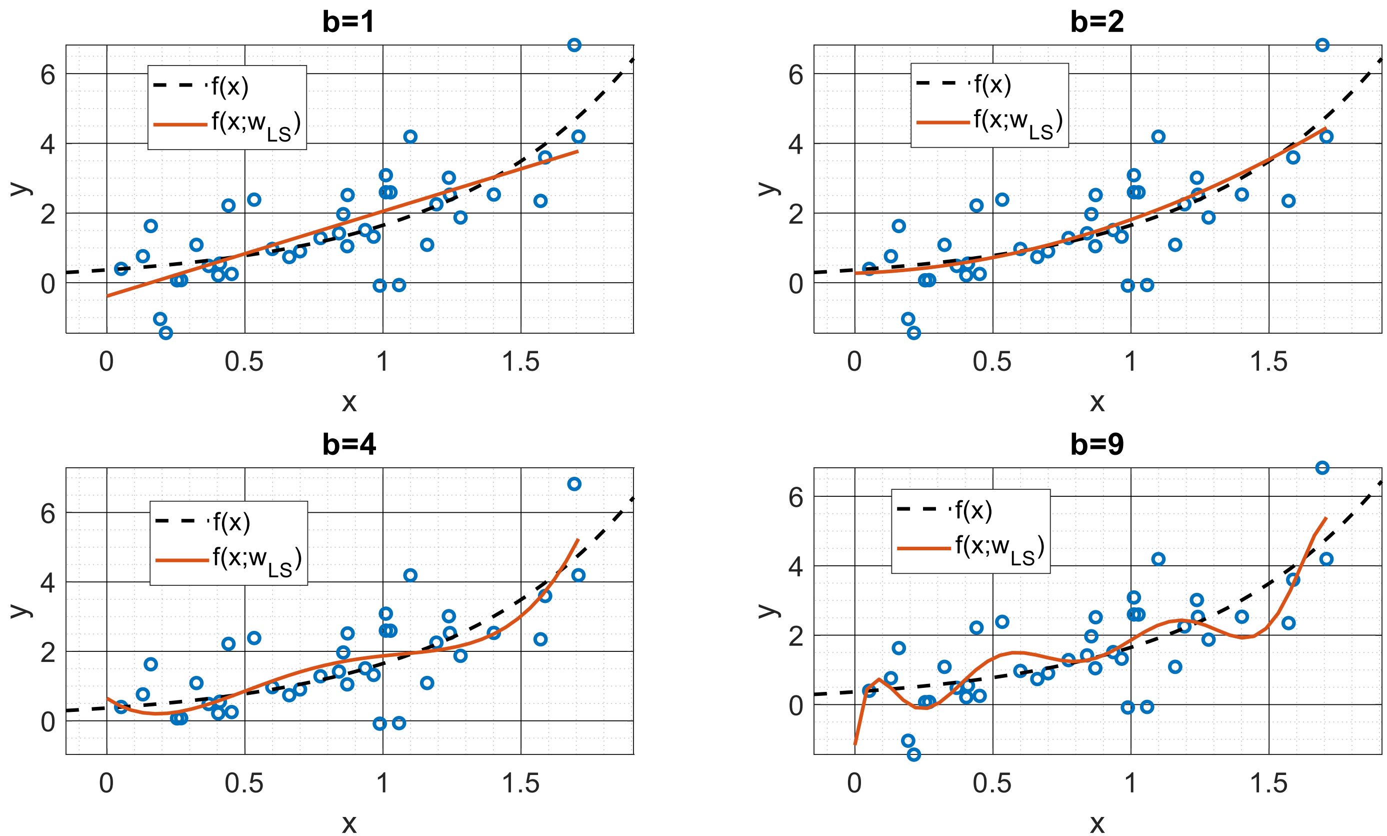
Today's class *roughly* follows Chapter 1.

Pattern Recognition and Machine Learning

Christopher Bishop, 2006

The Overfitting Issue…

- Last class, we faced a dilemma:
  - By using poly. feature, we can increase the flexibility of $f(\boldsymbol{x}; \boldsymbol{w})$.
  - The increased flexibility may also cause overfitting…



Overfitting and Regularization

- Large b causes overfitting
  - Pick a smaller b to avoid overfitting (using CV).
- What if we want to use a larger b?
  - We want the flexibility provided by high order polynomials.
- One trick we can do is called **regularization**.

$$\boldsymbol{w}_{\mathrm{LS-R}} := \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2 + \underbrace{\boxed{\lambda \boldsymbol{w}^\top \boldsymbol{w}}}_{\textbf{regularization term}}$$

- By adding a **regularization term** to LS Error.
- Note: $\lambda > 0$.

Overfitting and Regularization

$$\boldsymbol{w}_{\mathrm{LS-R}} := \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2 + \boxed{\lambda \boldsymbol{w}^\top \boldsymbol{w}}$$

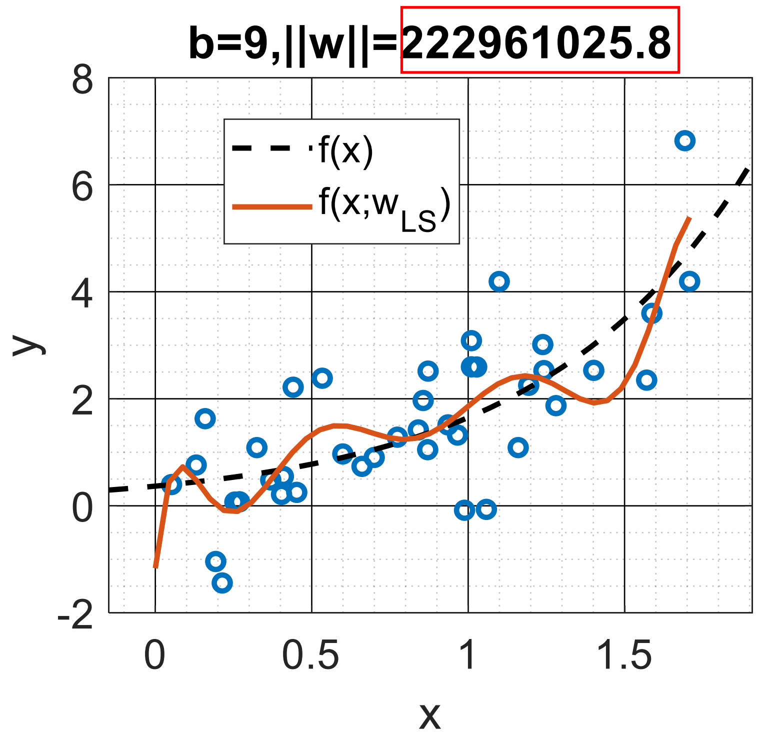
- $\boldsymbol{w}^\top \boldsymbol{w}$ is the magnitude of $\boldsymbol{w}$
- Regularization term discourages $\boldsymbol{w}$ taking large values.

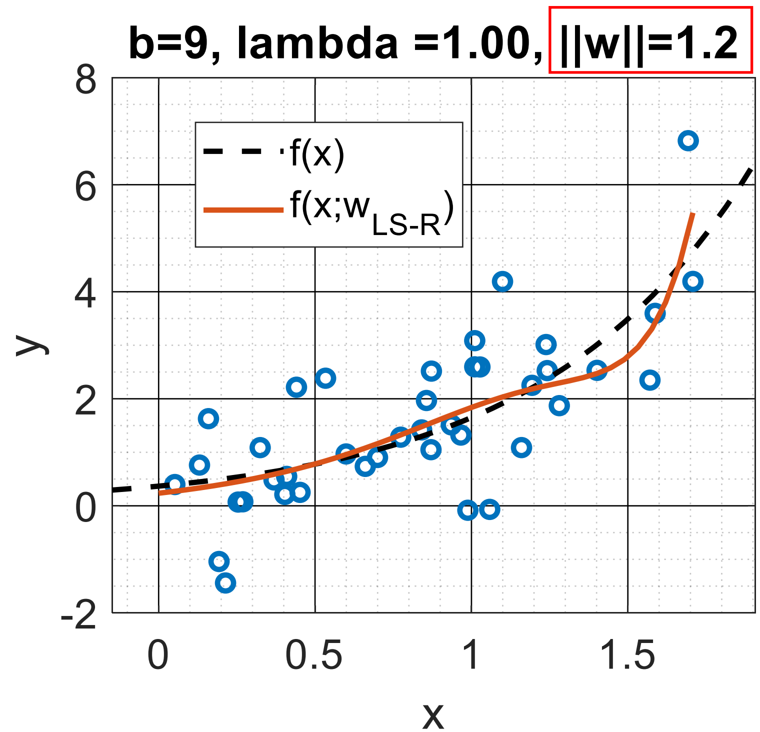
- Why does the regularization help overcome overfitting?

Overfitting and Regularization

- Prove that if regularization term is $\lambda \boldsymbol{w}^\top \boldsymbol{w}$,
- $\boldsymbol{w}_{\mathrm{LS-R}} \coloneqq (\boldsymbol{\phi}(\boldsymbol{X})\boldsymbol{\phi}(\boldsymbol{X})^\top + \lambda \boldsymbol{I})^{-1} \boldsymbol{\phi}(\boldsymbol{X})\boldsymbol{y}^\top$,
  - $\boldsymbol{I} \in R^{b \times b}$ is identity matrix.
- $\mathrm{limit}_{\lambda \to \infty} \boldsymbol{w}_{\mathrm{LS-R}} = \boldsymbol{0}$.
  - $\mathrm{limit}_{\lambda \to \infty} f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{LS-R}}) = 0$.
  - As you enlarge λ, coefficients in $\boldsymbol{w}_{\mathrm{LS-R}}$ get smaller and smaller.
  - As you enlarge λ, $f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{LS-R}})$ get flatter and flatter.
  - Which in turn reduces the complexity of $f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{LS-R}})$

Example





- $f(\boldsymbol{x}; w_{\mathrm{LS-R}})$ is much less squiggly than $f(\boldsymbol{x}; w_{\mathrm{LS}})$

See PRML, Table 1.2 for another example

Overfitting and Regularization

$$\boldsymbol{w}_{\mathrm{LS-R}} := \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2 + \boxed{\lambda \boldsymbol{w}^\top \boldsymbol{w}}$$

- Regularization term does not have to be $\boldsymbol{w}^\top \boldsymbol{w}$
- For example, $\sum_i |w_i|$, i.e. $||\boldsymbol{w}||_1$ can be used too!
- $||\boldsymbol{w}||_1$ and $\sqrt{\boldsymbol{w}^\top \boldsymbol{w}}$ are called "norms".

Norms

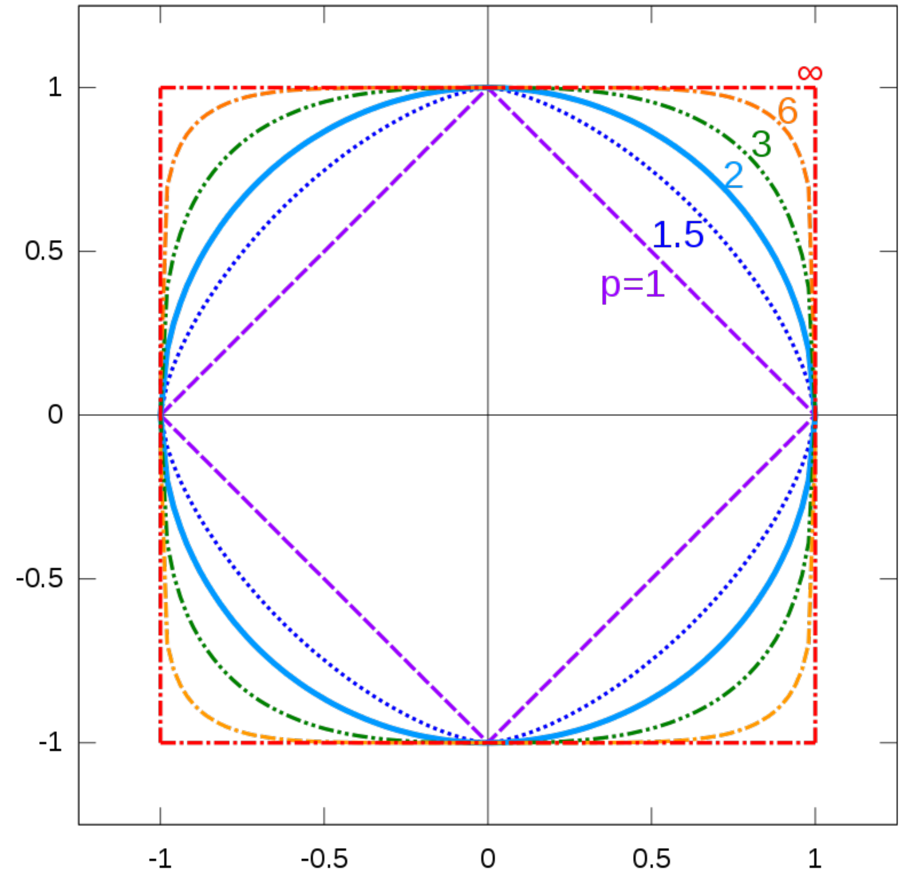
- Norms are widely used in machine learning.
- a generalization of the concept "length" in Euclidean spac.
  - $\sqrt{\boldsymbol{w}^{\top}\boldsymbol{w}}$ is the Euclidian distance from $\boldsymbol{w}$ to the origin.

- To become a norm, a function t must satisfy
  - If $t(\boldsymbol{x}) = 0$, then $\boldsymbol{x} = \mathbf{0}$
  - $t(\boldsymbol{x}) + t(\boldsymbol{y}) \geq t(\boldsymbol{x} + \boldsymbol{y})$, Triangle Inequality
  - $t(a \cdot \boldsymbol{x}) = |a| \cdot t(\boldsymbol{x})$

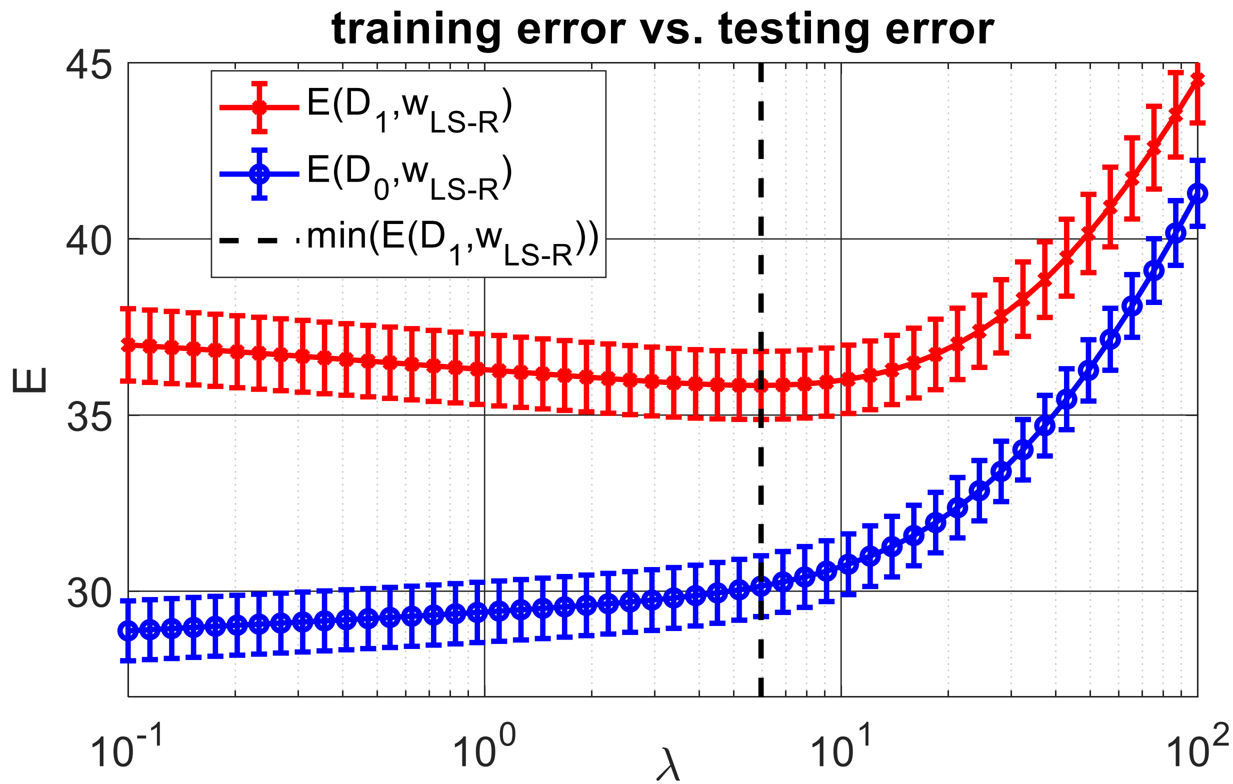
- Matrix cookbook, page 60, 61, 62.

L^p norms

- An important class of norms is called L^p norm.
- L^p norm for a real $p \geq 1$:
- $||\boldsymbol{x}||_p := (|x_1|^p + \cdots |x_d|^p)^{\frac{1}{p}}$
- Right: Unit "circle" defined by different L^p norms.



λ and Generalization



$D = D_0 \cup D_1$

D_0: Training set

D_1: Testing set

- Before the dash line, increasing λ reduces overfitting. After the dash line, increasing λ encourages underfitting.

See PRML, Figure 1.8

Problem of Regularization

- How do you choose λ?
- If we have plenty of i.i.d. data, we may choose a λ that minimizes the validation error using CV.
- However, what if we only have limited data.

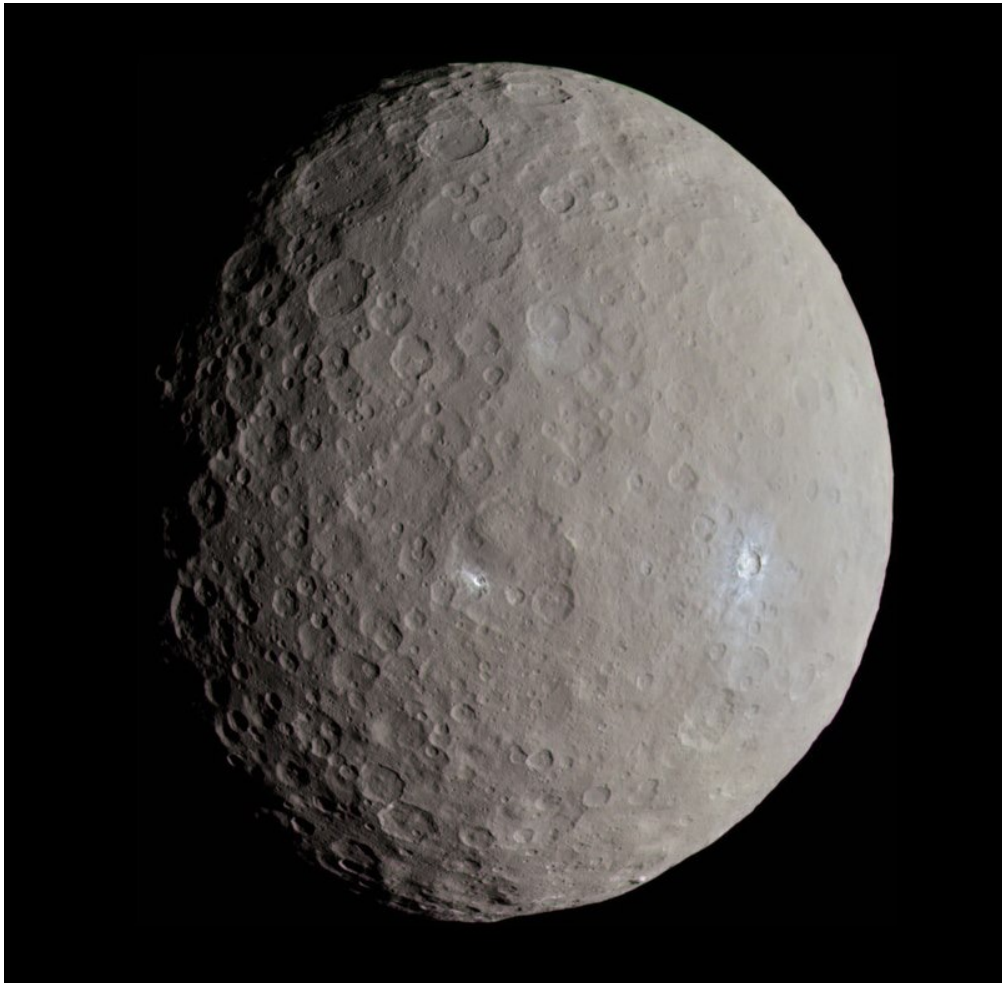
- Frequentist approach does not offer a straightforward way for tuning λ. To choose λ we need to adopt **a probabilistic view of regression problem.**

Inverse Problems

- Many data science problems are inverse problems.
- We have a dataset of noisy observations D
- We want to identify some **latent**, **unobserved** data generating mechanism.

- In regression, we observe y_i which is supposedly generated by
- $y_i = g(x_i) + \epsilon$, where ϵ is some noise.
- We are interested in finding the latent function g.

The Prediction of Ceres



Inverse Problems and Posterior

- The key of solving inverse problem is to infer posterior probability distributrion $p(g|D)$.
  - The word "posterior" comes from the fact that $p(g|D)$ is a probability obtained AFTER we observe D.
  - pp. 17, PRML
- The probability of a latent, data generating mechanism, g, given our dataset D.

- Problem: How do we obtain that posterior?

Bayes' Rule (or Law, Theorem)

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

- You can calculate a conditional probability given its "inverse probability".
- This theorem plays a key role in Bayesian statistics.
- Let us see how it helps us to obtain posterior $p(g|D)$.

Inverting the Posterior by Bayes' Rule

- Using Bayes' Rule, we know

$$\underbrace{p(g|D)}_{\text{Posterior}} = \frac{\overbrace{p(D|g)}^{\text{Likelihood}}\,\overbrace{p(g)}^{\text{Prior}}}{\underbrace{p(D)}_{\text{Evidence}}}$$

- $p(g)$ is called prior: the belief of our data generation mechanism g BEFORE the observation.
- $p(D|g)$ is called likelihood as it shows how likely we observe a specific dataset D given a data generator g.

Regression using Bayes' Rule

- In regression, we want to infer $p(g|D)$, where g is the data generating function:
- $y_i = g(\boldsymbol{x}_i) + \epsilon$.
- Suppose g admits a parametric form $g(\boldsymbol{x}) = f(\boldsymbol{x}; \boldsymbol{w})$, we only need to consider the parameter $\boldsymbol{w}$**.**
  - Once $\boldsymbol{w}$ is determined, f is determined.

- **Task:** Infer $p(\boldsymbol{w}|D)$
- **Bayes' Rule:** $p(\boldsymbol{w}|D) = \frac{p(D|\boldsymbol{w})p(\boldsymbol{w})}{p(D)}$

Regression using Bayes' Rule

- **Task:** Infer $p(\boldsymbol{w}|D)$
- **Bayes' Rule:** $p(\boldsymbol{w}|D) = \frac{p(D|\boldsymbol{w})p(\boldsymbol{w})}{p(D)}$
- If we assume ϵ is drawn from a Normal dist and D is IID:
- $p(D|\boldsymbol{w}) = \prod_{i \in D} p(y_i|\boldsymbol{x}_i, \boldsymbol{w}, \sigma^2) = \prod_{i \in D} N_{y_i}(f(\boldsymbol{x}_i; \boldsymbol{w}), \sigma^2)$

- To compute the Bayes' rule, we also need a prior $p(\boldsymbol{w})$.
- For now, we just use a Normal dist., $p(\boldsymbol{w}) = N_{\boldsymbol{w}}(0, \sigma_{\boldsymbol{w}}^2 \mathrm{I})$.

- $\boxed{p(\boldsymbol{w}|D) = \frac{\prod_{i \in D} N_{y_i}(f(\boldsymbol{x}_i; \boldsymbol{w}), \sigma^2) \cdot N_{\boldsymbol{w}}\left(0, \sigma_{\boldsymbol{w}}^2 \mathbf{I}\right)}{P(D)}}$

Maximum A Posteriori (MAP)

- $\boxed{p(\boldsymbol{w}|D) = \frac{\prod_{i \in D} N_{y_i}(f(\boldsymbol{x}_i; \boldsymbol{w}), \sigma^2) \cdot N_{\boldsymbol{w}}\left(0, \sigma_{\boldsymbol{w}}^2 \mathbf{I}\right)}{P(D)}}$
- How to make a prediction?
  - Find a $\boldsymbol{w}$ that is the most likely given our dataset D!
- To get a single $\boldsymbol{w}$, we can perform a maximization of $p(\boldsymbol{w}|D)$ with respect to $\boldsymbol{w}$.
- This procedure is called Maximum A Posteriori (MAP)
- $\boldsymbol{w}_{\text{MAP}} := \underset{\boldsymbol{w}}{\operatorname{argmax}}\, p(\boldsymbol{w}|D)$

$$= \operatorname{argmax}_{\boldsymbol{w}} \prod_{i \in D} N_{y_i}(f(\boldsymbol{x}_i; \boldsymbol{w}), \sigma^2) \cdot N_{\boldsymbol{w}}(0, \sigma_{\boldsymbol{w}}^2 \mathbf{I})$$

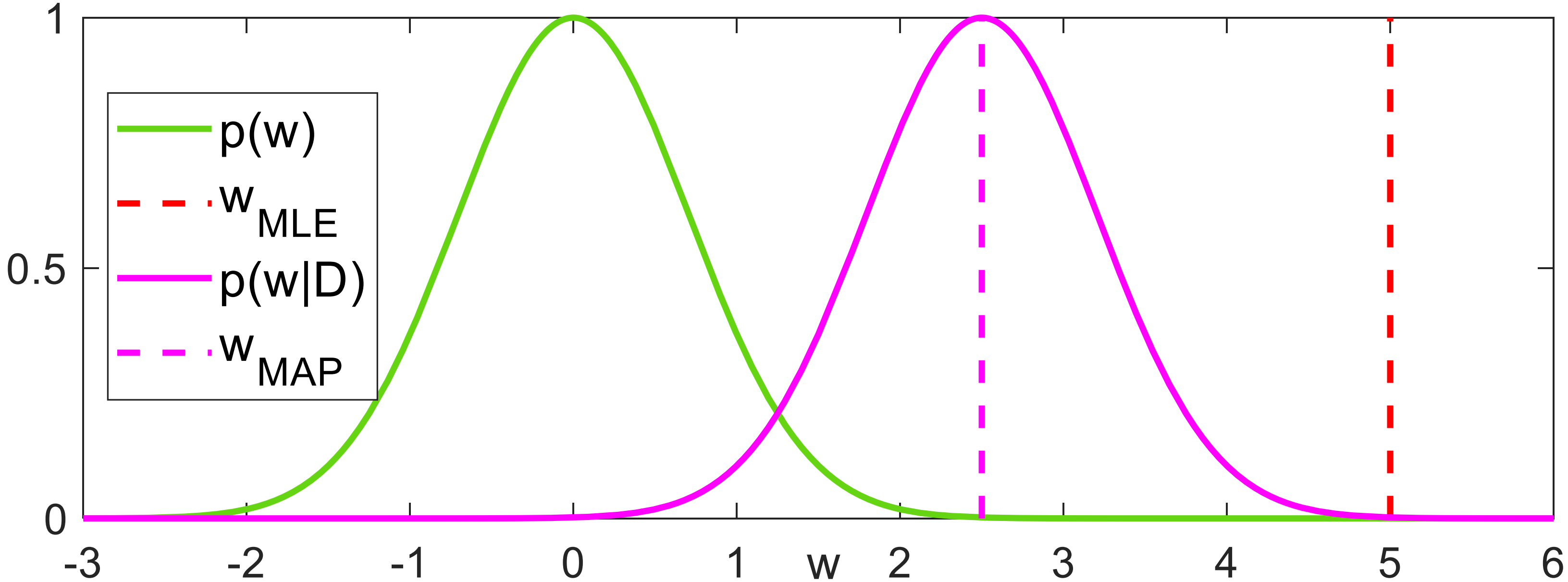
Maximum A Posteriori (MAP)

- Prove, $\mathbf{w}_{\mathrm{MAP}} = \boldsymbol{w}_{\mathrm{LS-R}}$ using $\lambda = \frac{\sigma^2}{\sigma_{\mathbf{w}}^2}$.

- After getting $\boldsymbol{w}_{\mathrm{MAP}}$, we can plug it in $f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{MAP}})$ to make predictions.

MAP vs. MLE

- $$\mathbf{w}_{\text{MAP}} = \underset{\boldsymbol{w}}{\operatorname{argmax}}\, p(\boldsymbol{w}|D) = \underset{\boldsymbol{w}}{\operatorname{argmax}}\, p(D|\boldsymbol{w})p(\boldsymbol{w})$$



A Full Probabilistic Approach

- However, why settle with a single $\boldsymbol{w}$ when you already have access to $p(\mathbf{w}|D)$?
- Using MAP to obtain a single $\boldsymbol{w}$ for prediction **ignores the uncertainty information** represented in $p(\mathbf{w}|D)$**.**

- If not getting a single $\boldsymbol{w}$, how do we make prediction using a probability $p(\mathbf{w}|D)$?

A Full Probabilistic Approach

- Instead of making a single prediction $\hat{y}$ given an $\boldsymbol{x}$.
- We can calculate the predictive distribution $p(\hat{y}|\boldsymbol{x}, D)$,
  - Probability of $\hat{y}$ given our dataset and $\boldsymbol{x}$.
- We know
- $p(\hat{y}|\boldsymbol{x}, D) = \int p(\hat{y}|\boldsymbol{x}, \boldsymbol{w})p(\boldsymbol{w}|D)d\boldsymbol{w}$, (why?)
- Calculate $p(\hat{y}|\boldsymbol{x}, D)$ as a marginalized probability.

- How can we calculate the predictive distribution?
- We can assume $p(\hat{y}|\boldsymbol{x}, \boldsymbol{w}) = N_{\hat{y}}(f(\boldsymbol{x}, \boldsymbol{w}), \sigma^2)$
- We can calculate $p(\boldsymbol{w}|D)$ up to a constant $p(D)$

Calculating Predictive Distribution

likelihood prior

- $p(\boldsymbol{w}|D) \propto \prod_{i\in D} N_{y_i}\left(f(\boldsymbol{x}_i;\boldsymbol{w}),\sigma^2\right) \cdot N_{\boldsymbol{w}}\left(0,\sigma_{\boldsymbol{w}}^2\mathbf{I}\right)$
- $p(\hat{y}|\boldsymbol{x},\boldsymbol{w}) = N_{\hat{y}}(f(\boldsymbol{x};\boldsymbol{w}),\sigma^2)$
- Suppose $f(\boldsymbol{x};\boldsymbol{w}) = \langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x})\rangle$
- **Prove:**
- $\int p(\hat{y}|\boldsymbol{x},\boldsymbol{w}) \cdot p(\boldsymbol{w}|D) d\boldsymbol{w} =$

$$N_{\hat{y}}\left[f(\boldsymbol{x};\boldsymbol{w}_{\mathrm{LS-R}}),\sigma^2 + \boldsymbol{\phi}^\top(\boldsymbol{x})\sigma^2\left(\boldsymbol{\phi}\boldsymbol{\phi}^\top + \frac{\sigma^2}{\sigma_{\boldsymbol{w}}^2}\boldsymbol{I}\right)^{-1}\boldsymbol{\phi}(\boldsymbol{x})\right]$$

- Where $\boldsymbol{\phi}$ is short for $\boldsymbol{\phi}(\boldsymbol{X})$, and $\boldsymbol{w}_{\mathrm{LS-R}}$ is the LS-R solution with $\lambda = \frac{\sigma^2}{\sigma_{\boldsymbol{w}}^2}$.

The Predictive Distribution

- $p(\hat{y}|\boldsymbol{x}, D) = \int p(\hat{y}|\boldsymbol{x}, \boldsymbol{w}) \cdot p(\boldsymbol{w}|D) d\boldsymbol{w} =$
$$N_{\hat{y}}\left[f(\boldsymbol{x}; \boldsymbol{w}_{\text{LS-R}}), \sigma^2 + \boldsymbol{\phi}^\top(\boldsymbol{x})\sigma^2\left(\boldsymbol{\phi}\boldsymbol{\phi}^\top + \frac{\sigma^2}{\sigma_{\boldsymbol{w}}^2}\boldsymbol{I}\right)^{-1}\boldsymbol{\phi}(\boldsymbol{x})\right]$$

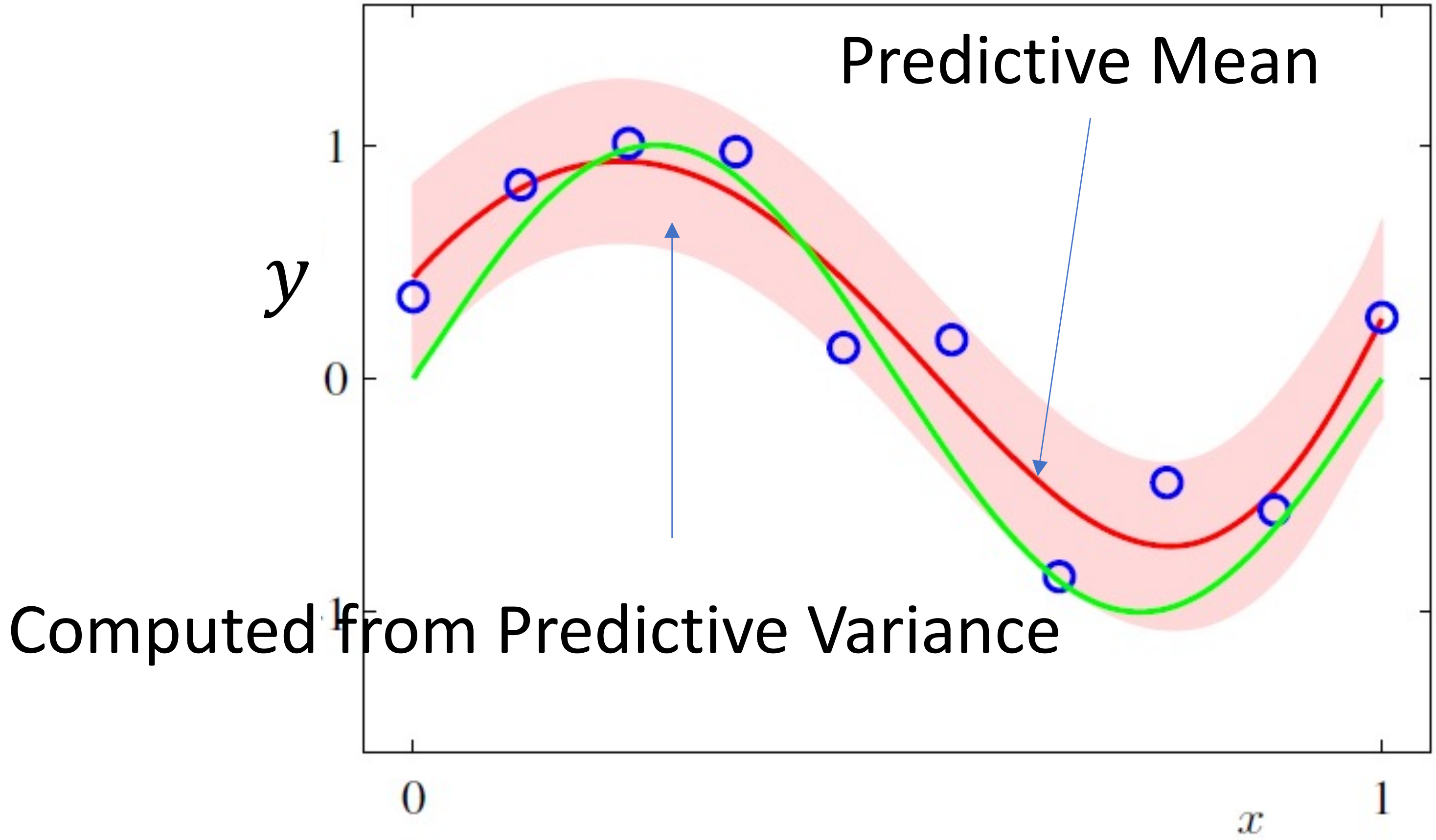
- The mean of $p(\hat{y}|\boldsymbol{x}, D)$ is the LS-R prediction!
- The idea of regularization naturally arises from both probabilistic modelling approaches.

A Full Probabilistic Approach

- With the predictive distribution $p(\hat{y}|\boldsymbol{x}, D)$, we can compute:
- Prediction: $\mathbb{E}_{p(\hat{y}|\boldsymbol{x}, D)}[\hat{y}|\boldsymbol{x}]$,
- Prediction uncertainty: $\mathrm{var}_{p(\hat{y}|\boldsymbol{x}, D)}[\hat{y}|\boldsymbol{x}]$.

- We can also use the predictive distribution to calculate other interesting expected values, as we will see later.

Example: $p(\hat{y}|x, D)$



- **PRML, Figure 1.17**

Conclusion

- We looked at "Regularized LS" from three different perspectives:
  - Regularized LS (Frequentist)
  - MAP (Semi-Bayesian)
  - Probabilistic Approach (Full Bayesian)

- However, we still have not incorporated an important concept, risk function, in our decision making process.
  - Recall, making wrong decisions has different consequences.
- Next, we talk about statistical decision making.
  - We will finally wrap up Chapter 1, PRML.

Homework

- Prove the statement on page 6
- Revisit: "The solution of $\boldsymbol{w}_{\mathrm{LS}}$ is useless if $n < d$."
  - Is this statement still true for $\boldsymbol{w}_{\mathrm{LS-R}}$?
- Prove the statement on page 21
- Prove the statement on page 25