The Basic of Statistical Learning

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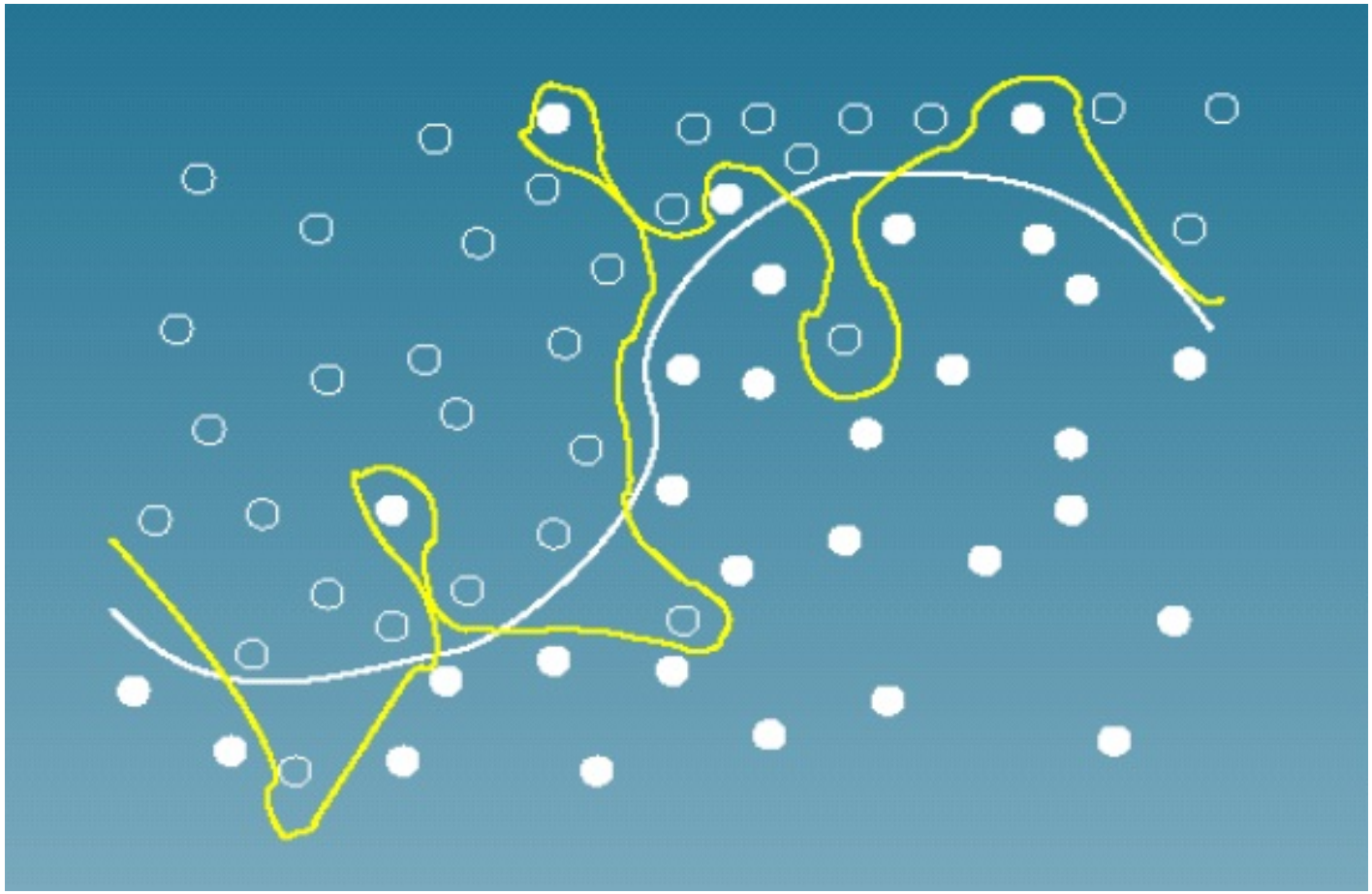
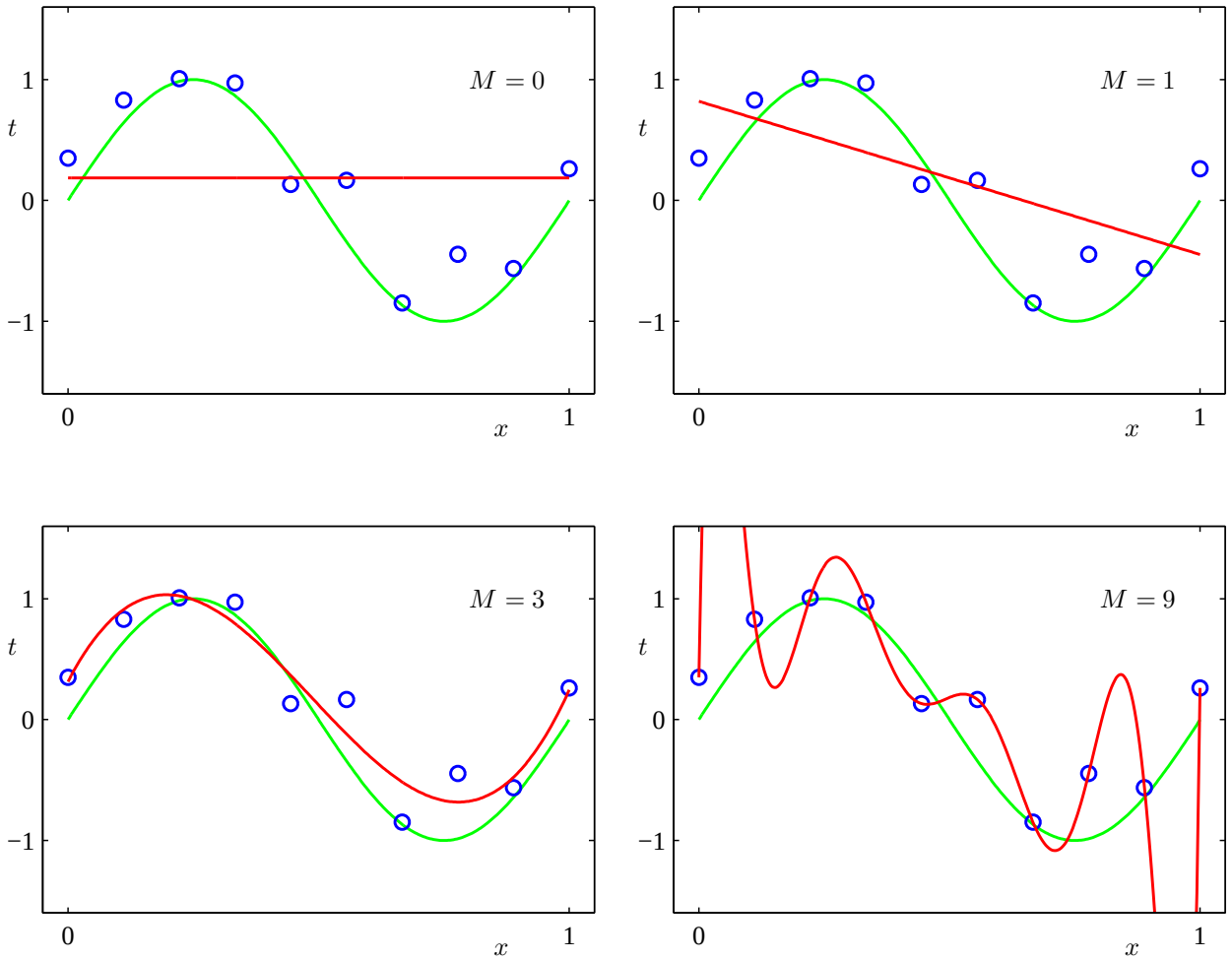
Outline I

Overfitting: k-NN



Overfitting: Regression



Training vs Testing

- Training data: $\mathcal{S} = \{(\mathbf{x}^{(1)}, y^{(1)}), ..., (\mathbf{x}^{(N)}, y^{(N)})\}$
- Test data: future observations that may be different from the training data
- Learning process:
  - learn prediction rule on training data
  - evaluate performance on test data
- Why separate training and testing?
  - training error is usually unrealistic low (overfitting)
  - error on test data (data not used to fit model) is more realistic

Training vs Testing (2)

- Goal: predict well on test data
- Two aspects:
  - model fit training data well
    - requires a more complex model
  - behavior of model on test data should match that on training data
    - requires a less complex (more stable) model
- Model complexity:
  - more complex model: smaller training error but larger difference between test and training error
  - less complex model: larger training error but smaller difference between test and training error

Regularization: A Technique Toward Overfitting

- Training error(f) = $\frac{1}{N}\sum_{i=1}^{N}(f(\mathbf{x}^{(i)}) - y^{(i)})^2$
- Test error(f) = $\mathbb{E}_{(\mathbf{x},y)}[f(\mathbf{x}) - y]^2$
- Model complexity: the difference between training and test error
  - increase model complexity decreases training error but increases difference between training and test
- Generalization: the ability to categorize correctly new samples that differ from those used for training.
- Regularization allows complex models to be trained on data sets of limited size without severe ovefitting, by limiting the effective model complexity.
- Benefits of regularization:
  - statistical: robust to large number of features
  - numerical: stabilize solution

Regularized Linear Regression

- Regularized error of least squares regression:

$$\frac{1}{2}\sum_{i=1}^{N}(\mathbf{w}^T\mathbf{x}^{(i)} - y^{(i)})^2 + \frac{\lambda}{2}\sum_{j=1}^{D}|w_j|^p$$

  - $\lambda \geq 0$ is the regularization parameter
  - $p = 0$: subset selection, non-convex, non-smooth
  - $p \in (0, 1)$: non-convex, smooth
  - $p \geq 1$: convex
  - $p = 1$: Lasso
  - $p = 2$: ridge repression
- Model complexity: small $\lambda \rightarrow$ large complexity

Ridge Regression

Regularization formulation:

$$\hat{\mathbf{w}}_{ridge} = \arg\min_{\mathbf{w}\in\mathbb{R}^D} \sum_{i=1}^{N} (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)})^2 + \lambda \sum_{j=1}^{D} |w_j|^2$$

.

- Implicit dimension reduction (the loadings can be recovered by regressing the principal component on D variable)
- More stable (smaller weight) than least squares
- It does not generally lead to sparse solution.
- Closely related to kernel method

Solution of Ridge Regression

- Denote $\mathbf{X} = [\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}] \in \mathbb{R}^{D \times N}$,$\mathbf{y} = [y^{(1)}, \ldots, y^{(N)}] \in \mathbb{R}^{N}$.
- Solution of ridge regression:

$$\hat{\mathbf{w}}_{ridge} = (\mathbf{X}\mathbf{X}^T + \lambda \mathbf{I})^{-1}\mathbf{X}\mathbf{y}$$

.

- Compared to standard least square regression solution:

$$\hat{\mathbf{w}} = (\mathbf{X}\mathbf{X}^T)^{-1}\mathbf{X}\mathbf{y}$$

- Advantage: ridge regression allows $D > N$
  - stable: $\mathbf{X}\mathbf{X}^T + \lambda \mathbf{I}$ is always invertible
  - implicit dimension reduction

Lasso

Regularization formulation:

$$\hat{\mathbf{w}}_{lasso} = \arg\min_{\mathbf{w}\in\mathbb{R}^D} \sum_{i=1}^{N} (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)})^2 + \lambda \sum_{j=1}^{D} |w_j|$$

.

- Originally proposed in [Tib96], lasso for "least absolute shrinkage and selection operator".
- Convex optimization problem, but solution may not be unique.
- Global solution can be efficiently found (e.g., by Least Angle Regression (LARS) [EHJT04]).
- Solution is sparse, achieving feature selection.
- Solutionis not necessarily stable.

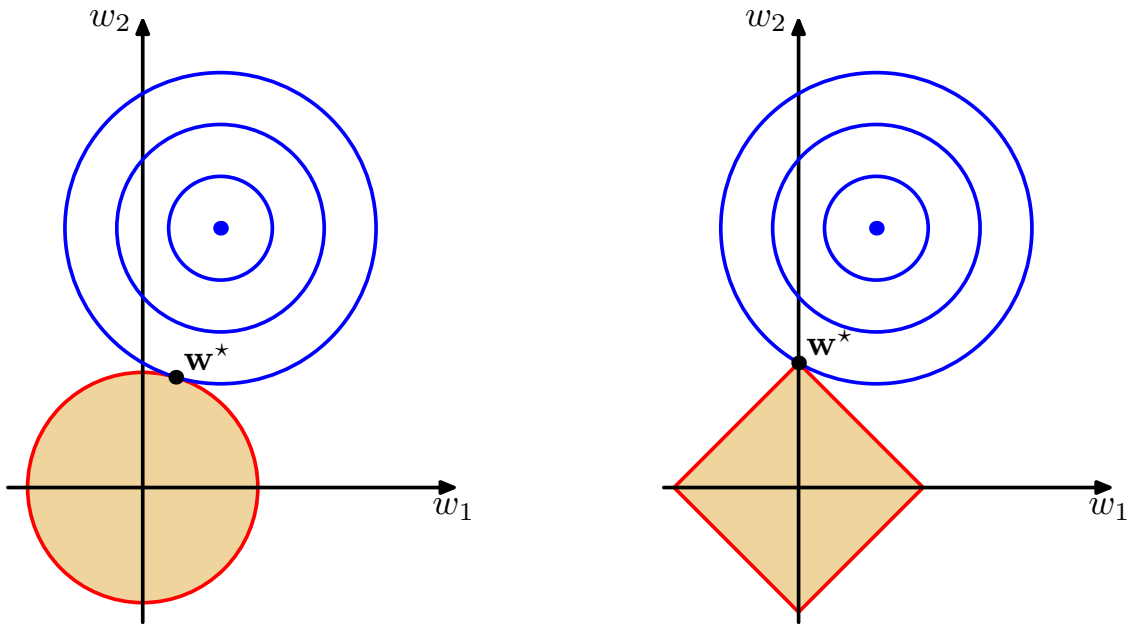
More on Lasso

- Limitation of lasso: the number of selected variables by the lasso is limited by the number of observations N.
  - E.g., for microarray data where there are thousands of genes but less than 100 samples
- Elastic net [ZH03]:

$$\hat{\mathbf{w}}_{en} = \arg\min_{\mathbf{w}\in\mathbb{R}^D} \sum_{i=1}^{N}(\mathbf{w}^T\mathbf{x}^{(i)} - y^{(i)}) + \lambda_2 \sum_{j=1}^{D} |w_j|^2 + \lambda_1 \sum_{j=1}^{D} |w_j|$$

  - Elastic net has grouping effect, i.e., it tends to select a group of highly correlated variables once one variable among them is selected.
  - Lasso tends to select only one out of the grouped variables and does not care which one is in the final model.

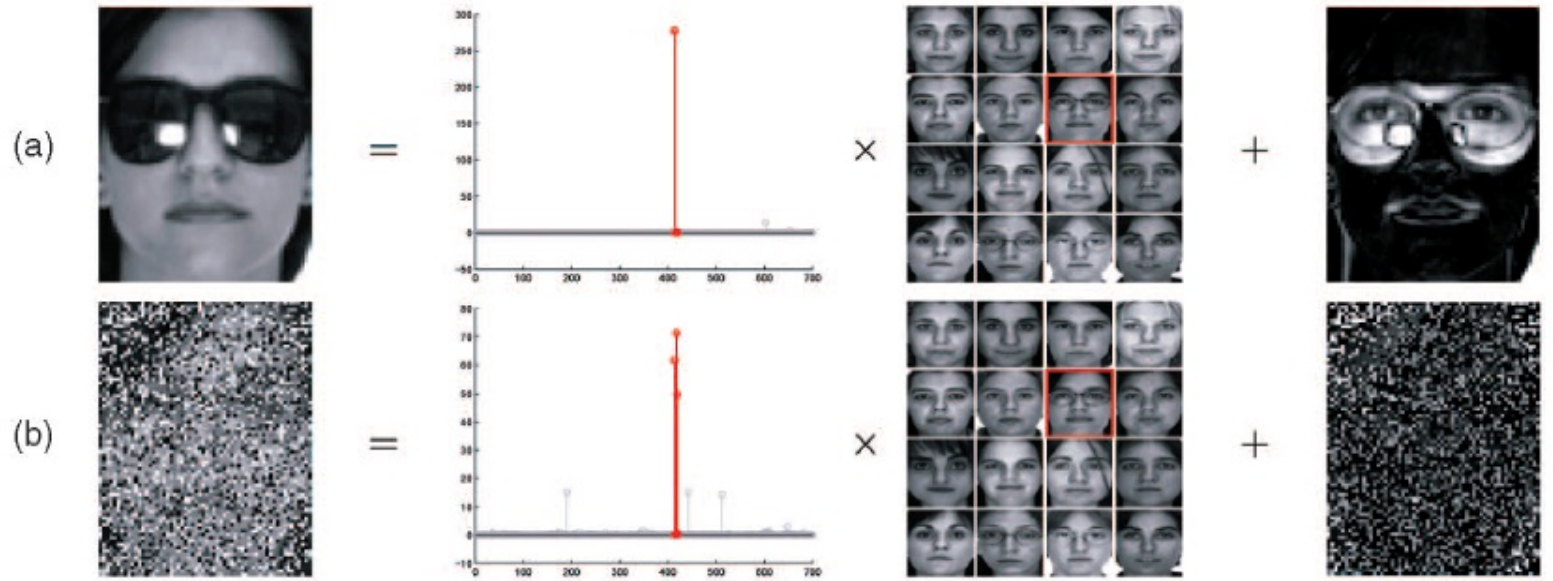
The effect of *L1* and *L2* Norms



- (left) Using the L_2 norm pulls directly towards the origin.
- (right) Using the L_1 norm pulls towards the coordinate axes, i.e., it tries to set some of the coordinates to 0.

Applications with Sparse Representation

- Robust face recognition



- Image super-resolution/inpainting/deblur
- Robust visual tracking
- More useful with lasso extensions:
  - tree-guided group lasso
  - graph-guided fused lasso
  - etc.

Generalization error

- Generalization error of a hypothesis: its expected error on examples not necessarily in the training set
- Informally,
  - Bias of a model is the expected generalization error even if we were to fit it to a very large training set.
  - Variance of a model is brought by the "spurious" samples in the training set.
  - "Simple" models with few parameters may have large bias (but small variance); "complex" models with many parameters may have large variance (but small bias).

Bias-variance Decomposition

- A frequentist viewpoint of the model complexity issue [GBD92][Fri97]
- Denote:
  - $f(\mathbf{x}; \mathcal{D})$ as the prediction function trained on data set $\mathcal{D}$
  - $h(\mathbf{x})$ as the optimal prediction
- Expected loss of least square regression:

$$\begin{aligned}\mathbb{E}[L] &= \int\int (f(\mathbf{x}) - y)^2 p(\mathbf{x}, y) d\mathbf{x} dy \\ &= \int (f(\mathbf{x}) - h(\mathbf{x}))^2 p(\mathbf{x}) d\mathbf{x} + \int\int (h(\mathbf{x}) - y)^2 p(\mathbf{x}, y) d\mathbf{x} dy\end{aligned}$$

  - $h(\mathbf{x}) = \mathbb{E}[y|\mathbf{x}]$. Given unlimited supply of data, we could in principle find $h(\mathbf{x})$ to any degree of accuracy, which is the optimal choice of $f(\mathbf{x})$. For finite dataset, we do not know $h(\mathbf{x})$ exactly.
  - The second term, which is independent of $f(\mathbf{x})$, arises from the intrinsic noise on the data.

Bias-variance Decomposition (2)

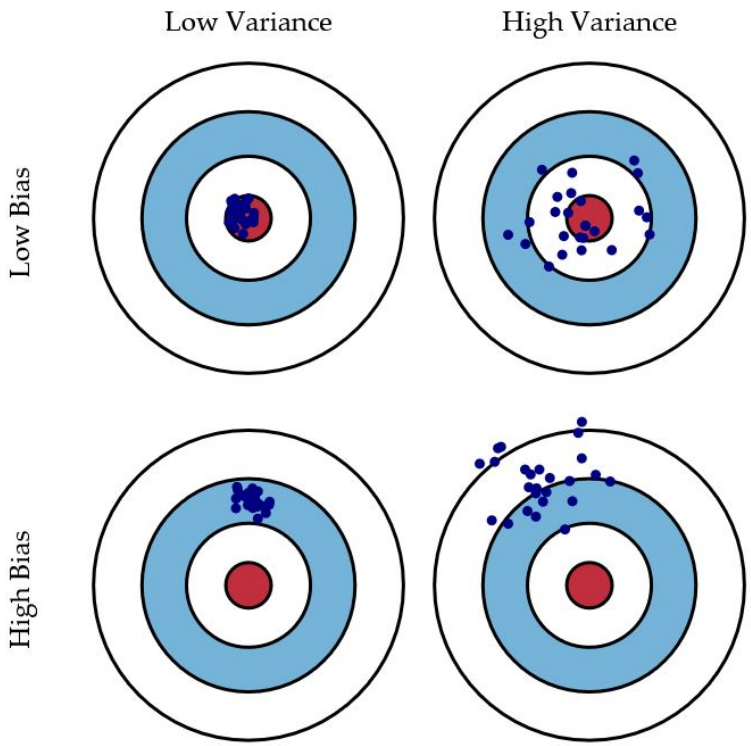
- For particular dataset $\mathcal{D}$:

$$\begin{aligned} & \mathbb{E}_{\mathcal{D}}[(f(\mathbf{x};\mathcal{D}) - h(\mathbf{x}))^2] \\ = \; & (\mathbb{E}_{\mathcal{D}}[f(\mathbf{x};\mathcal{D})] - h(\mathbf{x}))^2 + \mathbb{E}_{\mathcal{D}}[(f(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\mathbf{x};\mathcal{D})])^2] \\ = \; & (\mathit{bias})^2 + \mathit{variance} \end{aligned} \tag{1}$$

  - $\mathbb{E}_{\mathcal{D}}$ means take the average over the ensemble of data sets.
  - The squared bias represents the extent to which the average prediction over all data sets differs from the desired regression function.
  - The variance measures the extent to which the solutions for individual data sets vary around their average, the extent to which the function $f(\mathbf{x};\mathcal{D})$ is sensitive to the particular choice of data set.
- Expected loss = $(\text{bias})^2$ + variance + noise

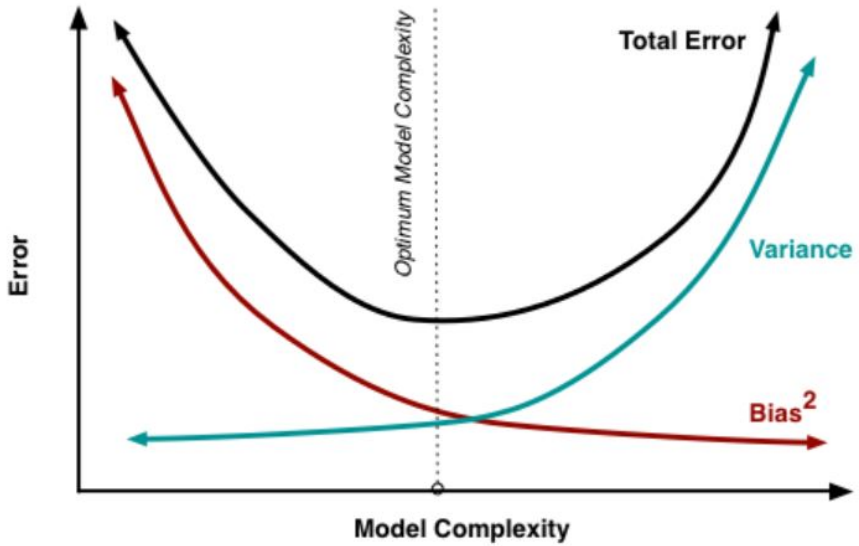
Intuitive Explanation

- Graphical illustration of bias and variance



Intuitive Explanation

- Bias and variance contributing to total error



An Example

- 100 independent data sets $\mathcal{D}^{(l)}, l = 1, \ldots, 100$, each containing $N = 25$ data points, generated from $\sin(2\pi x)$.
- Model:
  - Linear regression with 24 Gaussian basis functions

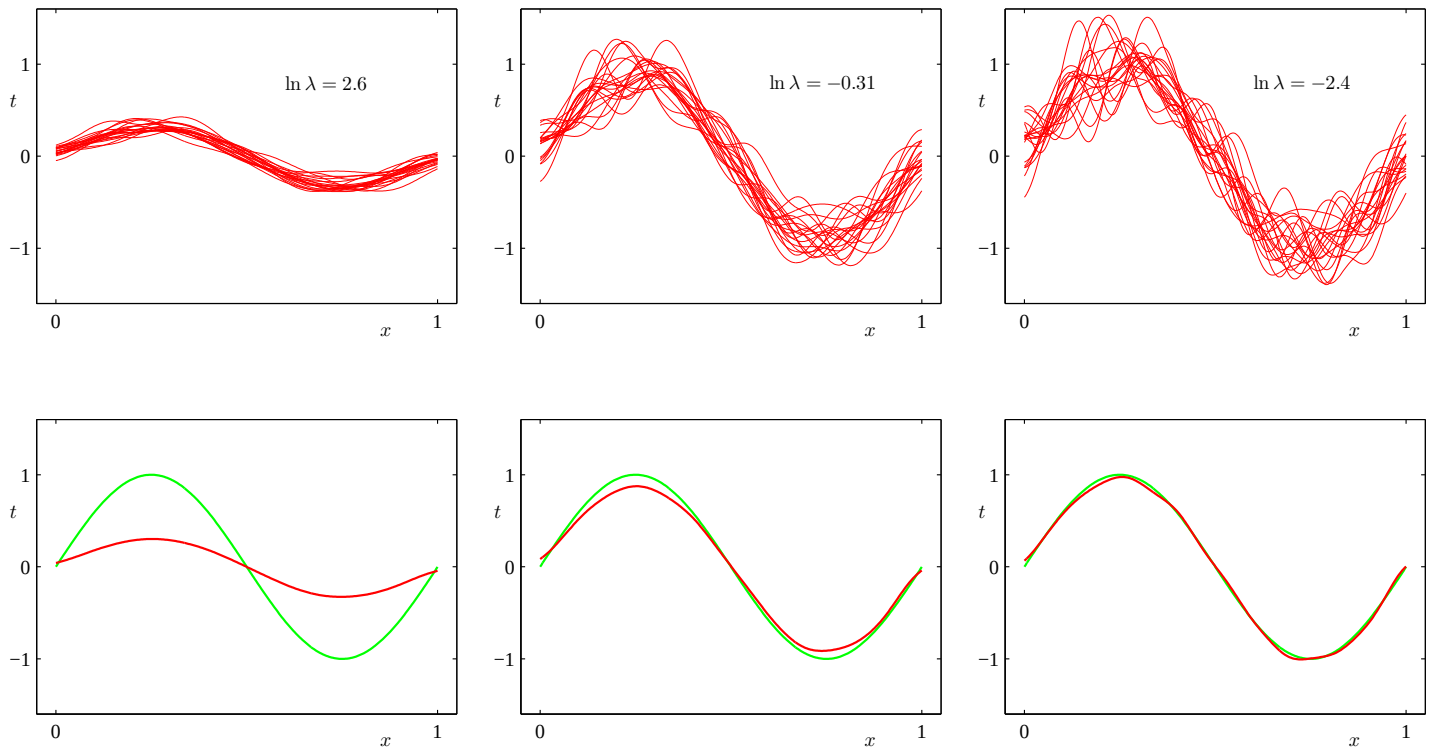
$$f(\mathbf{x}; \mathbf{w}) = w_0 + \sum_{j=1}^{24} w_j \phi_j(\mathbf{x}),$$

    where $\phi_j(\mathbf{x}) = \exp(-(\mathbf{x} - \boldsymbol{\mu}_j)^2/2s)$.
  - regularized least square error:

$$\sum_{i=1}^{N} (y^{(i)} - \mathbf{w}^T \Phi(\mathbf{x}^{(i)}))^2 + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w}$$

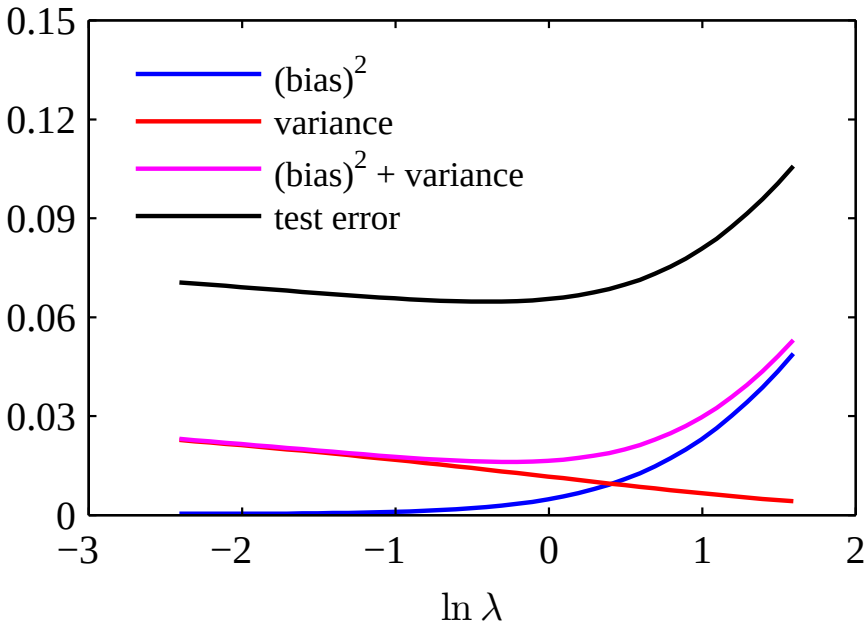
An Example

- Illustration of the dependence of bias and variance on model complexity, governed by regularization parameter λ



An Example

- Test set error for a test data set size of 1000 points



- Small λ allows the model to become finely tuned to the noise on each individual data set, leading to large variance.
- Large λ pulls the weight parameters towards zeros, leading to large bias.

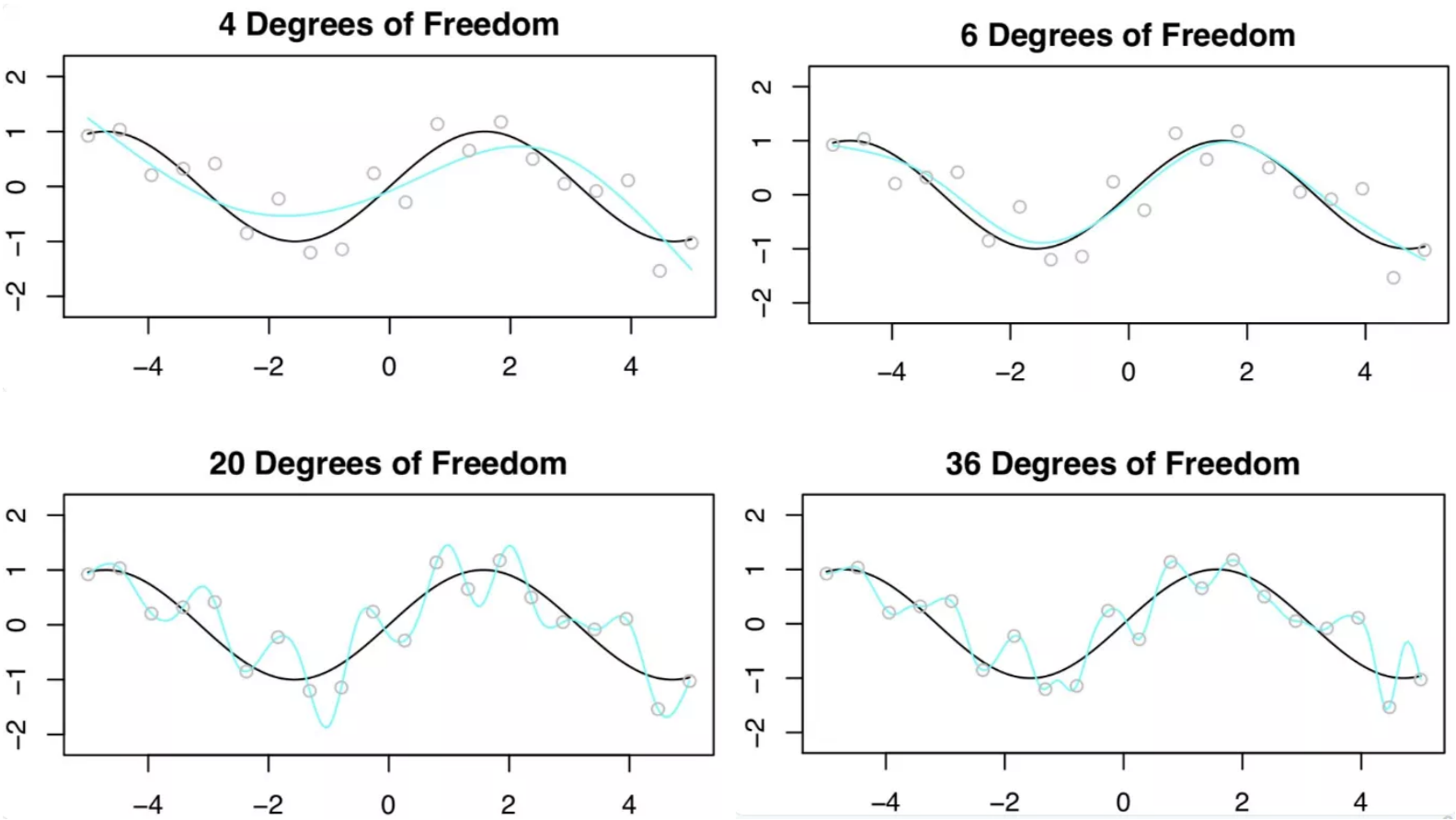
Bias-variance Tradeoff

- A good insight into model complexity issue:
  - Very flexible models having low bias and high variance
  - Relatively rigid models having high bias and low variance.
  - The model with the optimal predictive capability is the one that leads to the best balance between bias and variance.
- More discussions:
  - A bit of variance may be a good thing.
    - E.g., bias-corrected lease square estimator.
  - We sometimes would like to pay a little bias to save a lot of variance.
    - We can pay in model bias, or estimation bias.
    - Less rich model: model bias up, but less parameters to estimate (Feature selection)
    - Prefer well-behaved functions despite poorer fit: more estimation bias, lower variance (Regularization)

However ...

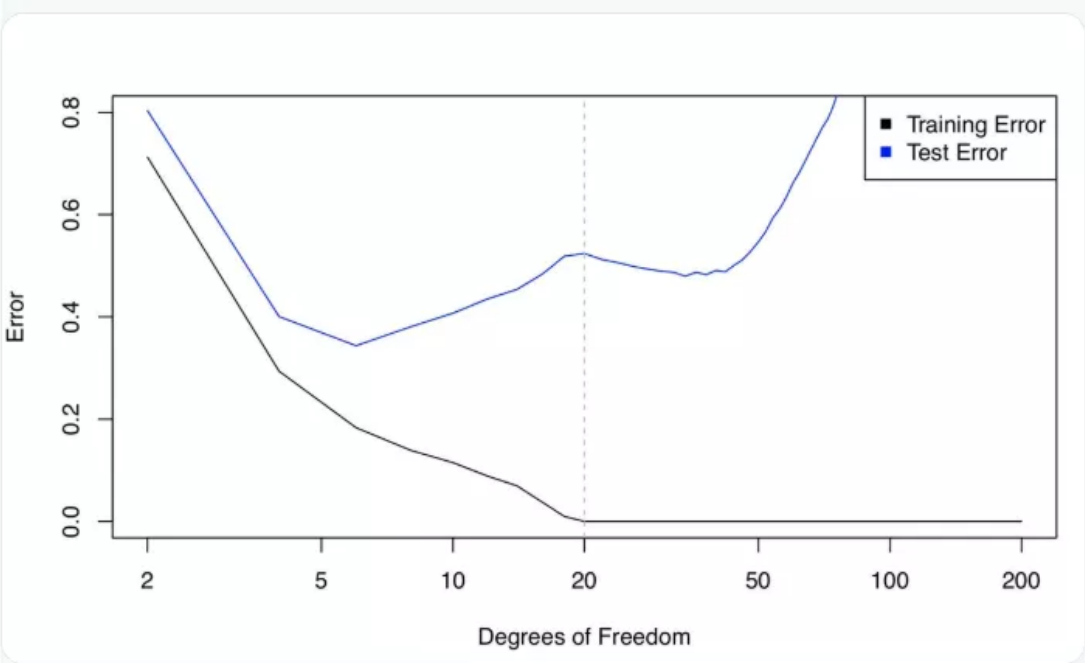
- Bias-variance decomposition has limited practical value
  - Bias and variance cannot be computed since it relies on knowing the true distribution of $\mathbf{x}$ and y(and hence $h(\mathbf{x}) = \mathbb{E}[y|\mathbf{x}]$).
  - Bias-variance decomposition is based on averages with respect to ensembles of data sets, whereas in practice we have only the single observed data set.
- Bayesian model selection
  - Frequentist view: parameters are constant-valued but unknown
  - Bayesian view: parameters are random variables

Another Example



- Fitting with cubic spline, $N = 20$, degree of freedom = ♯ basis functions

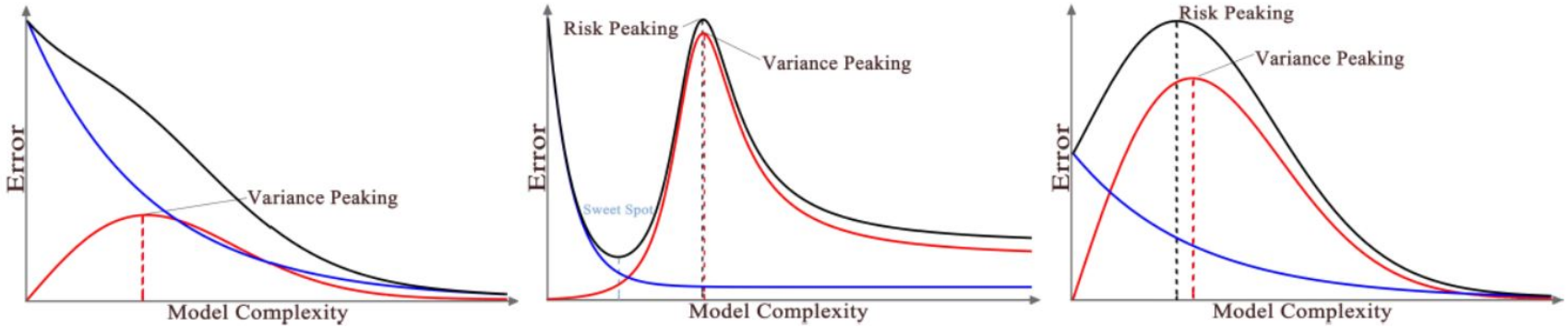
Double Descent Curve



- Why double descent curve should occur?
- Fitting with minimum norm

Generalization of Neural Networks

- Typical cases of expected risk curve (in black) in neural networks [ZY20].



  - squared bias, variance
  - The risk displays one of the three patterns: monotonically decreasing, double descent, and unimodal.
  - Label noise may increase the variance of the model and hence lead to double-descent risk.

A Few Questions

- How to explain bias variance tradeoff in statistical learning theory?
- How to relate training error to generalization error?
  - We care about generalization error,
  - but we fit models to the training set.
  - The goal is to estimate the difference of generalization error and training error.
- How good is the learning algorithm compared to the best possible prediction rule in a class?
- Are there conditions under which we can actually prove that the learning algorithms will work well?

Training and Generalization Error

- Training error (for binary classification):

$$\hat{\varepsilon}(f) = \frac{1}{N} \sum_{i=1}^{N} 1\{f(\mathbf{x}^{(i)}) \neq y^{(i)}\}$$

- Generalization error:

$$\varepsilon(f) = \mathbb{E}_{(\mathbf{x},y)}[1\{f(\mathbf{x}) \neq y\}]$$

  - Assumption: training and testing on the same distribution (one of PAC assumptions).
- Empirical risk minimization (ERM):
  - The most basic learning strategy
  - For $f_{\mathbf{w}}(\mathbf{x}) = 1\{\mathbf{w}^T\mathbf{x} \geq 0\}$, the ERM gives $\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \hat{\varepsilon}(f_{\mathbf{w}})$.

ERM Over Hypothesis Class

- Hypothesis class $\mathcal{H}$ is the set of all classifiers considered by a learning algorithm.
  - For linear classification, $\mathcal{H} = \{f_{\mathbf{w}} : f_{\mathbf{w}} = 1\{\mathbf{w}^T\mathbf{x} \geq 0\}, \mathbf{w} \in \mathbb{R}^{D+1}\}$.
- Empirical risk minimization selects $\hat{f}$ to be the hypothesis with the smallest training error.

$$\hat{f} = \arg\min_{f \in \mathcal{H}} \hat{\varepsilon}(f)$$

- How about the generalization error of $\hat{f}$?
  - $\hat{\varepsilon}(f)$ is a reliable estimate of $\varepsilon(f)$.
  - This implies an lower-bound on the generalization error of $\hat{f}$.

The Case of Finite H

- $\mathcal{H} = \{f_1, \ldots, f_k\}$
- For particular f_i, training error is close to generalization error with high probability, assuming N ($\sharp$ training examples) is large.

$$P(|\varepsilon(f_i) - \hat{\varepsilon}(f_i)| > \gamma) \leq 2e^{-2\gamma^2 N}$$

- For all $f \in \mathcal{H}$, we get uniform convergence result:

$$P(\forall f \in \mathcal{H}, |\varepsilon(f) - \hat{\varepsilon}(f)| \leq \gamma) \geq 1 - 2ke^{-2\gamma^2 N}$$

The Case of Finite H (2)

- Given $\gamma, \delta > 0$, if $N \geq \frac{1}{2\gamma^2} \log \frac{2k}{\delta}$, with probability at least $1 - \delta$, we have $|\varepsilon(f) - \hat{\varepsilon}(f)| \leq \gamma$ for all $f \in \mathcal{H}$.
  - setting $\delta = 2ke^{-2\gamma^2 N}$
  - definition of sample complexity bound
- Given N, δ, with probability at least $1 - \delta$, we have for all $f \in \mathcal{H}$,

$$|\varepsilon(f) - \hat{\varepsilon}(f)| \leq \sqrt{\frac{1}{2N} \log \frac{2k}{\delta}}.$$

The Case of Finite H (3)

- Define $f^* = \arg\min_{f \in \mathcal{H}} \varepsilon(f)$, the best possible hypothesis in $\mathcal{H}$
- Our learning algorithm picks $\hat{f} = \arg\min_{f \in \mathcal{H}} \hat{\varepsilon}(f)$.
- Comparing $\hat{f}$ with f^*:

$$\begin{aligned} \varepsilon(\hat{f}) &\leq \hat{\varepsilon}(\hat{f}) + \gamma \\ &\leq \hat{\varepsilon}(f^*) + \gamma \\ &\leq \varepsilon(f^*) + 2\gamma \end{aligned}$$

  - If uniform convergence holds, the generalization error of $\hat{f}$ is at most 2γ worse than the best possible hypothesis in $\mathcal{H}$.

Relation to Bias/Variance Tradeoff

Theorem

Given $|\mathcal{H}| = k, N$ and δ fixed, with probability at least $1 - \delta$, we have that

$$\varepsilon(\hat{f}) \leq (\min_{f \in \mathcal{H}} \varepsilon(f)) + 2\sqrt{\frac{1}{2N} \log \frac{2k}{\delta}}$$

- Suppose we switch from $\mathcal{H}$ to some larger hypothesis class $\mathcal{H}' \supseteq \mathcal{H}$, then
  - The first term decreases. The "bias" decreases.
  - The second term increases (with larger k). The "variance" increases.
- By holding γ and δ fixed and solving for N, we can get sample complexity bound.

VC Dimension

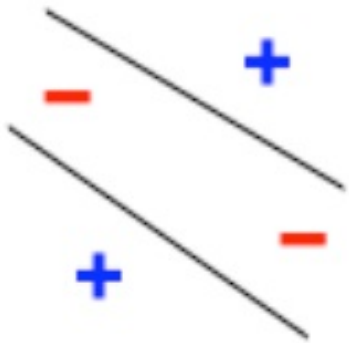
- Shattering: A function class $\mathcal{H}$ is said to shatter a set of data points $(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)})$ if $\mathcal{H}$ can realize any labeling on this data set, i.e., for every assignment of labels to those points $(y^{(1)}, \ldots, y^{(N)})$, there exists a function $f \in \mathcal{H}$ such that f makes no errors when evaluating that set of data points: $f(\mathbf{x}^{(i)}) = y^{(i)}$ for all i.

VC dimension

VC dimension $VC(\mathcal{H})$ is the size of the largest data set that can be shattered by $\mathcal{H}$.

VC Dimension - An Example

- Consider $\mathcal{H} = \{1(\mathbf{w}^T\mathbf{x} + b \geq 0)\}$ ($\mathbf{w} \in \mathbb{R}^2, b \in \mathbb{R}$), a set of binary linear classifiers in 2-D space.
- There exist 3 points $[0,0], [0,1], [1,0]$ that can be shattered by $\mathcal{H}$.
- Any four points cannot be shattered.



- So the VC dimension is 3.
- More general: D-dimensional linear classifier has VC dimension of $D+1$.

The Case of Infinite H

Theorem

Given $\mathcal{H}$, and let $D = VC(\mathcal{H})$. Then with probability at least $1 - \delta$, we have for all $f \in \mathcal{H}$,

$$|\varepsilon(f) - \hat{\varepsilon}(f)| \leq O(\sqrt{\frac{D}{N}\log\frac{N}{D} + \frac{1}{N}\log\frac{1}{\delta}}).$$

Thus, with probability at least $1 - \delta$, we also have

$$\varepsilon(\hat{f}) \leq \varepsilon(f^*) + O(\sqrt{\frac{D}{N}\log\frac{N}{D} + \frac{1}{N}\log\frac{1}{\delta}}).$$

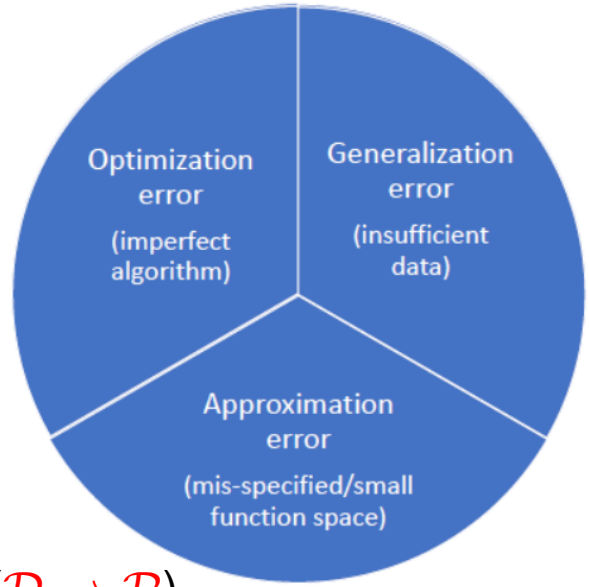
- If a hypothesis class has finite VC dimension, then uniform convergence occurs as N becomes large.

The Case of Infinite H (2)

- Corollary: For $|\varepsilon(f) - \hat{\varepsilon}(f)| \leq \gamma$ to hold for all $f \in \mathcal{H}$ (and hence $\varepsilon(\hat{f}) \leq \varepsilon(f^*) + 2\gamma$) with probability at least $1 - \delta$, it suffices that $N = O_{\gamma,\delta}(D)$.
  - The number of training examples needed to learn "well" using $\mathcal{H}$ is linear in the VC dimension of $\mathcal{H}$.
- For most hypothesis classes, the VC dimension is roughly linear in the number of parameters.
- Therefore, the number of training examples needed is roughly linear in the number of parameters of $\mathcal{H}$.

Statistical Learning Theory

- Reality: Find a function f from a hypothesis class $\mathcal{F}$ based on training data set $\mathcal{D}$
- Goal: f performs well on test data from a distribution $\mathcal{P}$



- Where is the gap:
  - generalization error ($\mathcal{D} \to \mathcal{P}$)
  - approximation error (Hypothesis space $\mathcal{F}$)
  - optimization error (How to find)

Decomposition of Learning Error

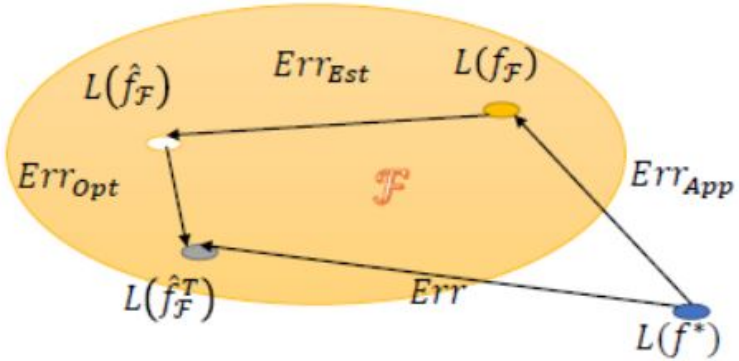
- Definition:
  - Training data: $\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(N)}, y^{(N)})\}$
  - Model: $f \in \mathcal{F}$
  - Loss: $l(f(\mathbf{x}), y)$
  - Risk: $L(f) = \mathbb{E}[l(f(\mathbf{x}), y)]$
  - Empirical risk: $\hat{L}(f) = \frac{1}{N} \sum_{i=1}^{N} l(f(\mathbf{x}^{(i)}), y^{(i)})$
  - Bayes risk: $L^* = \min_f \mathbb{E}[l(f(\mathbf{x}), y)]$
  - Solutions:

$$
\begin{aligned}
f^* &= \arg\min_f \mathbb{E}[l(f(\mathbf{x}), y)] \quad \text{(Bayes prediction function)} \\
f_{\mathcal{F}} &= \arg\min_{f \in \mathcal{F}} \mathbb{E}[l(f(\mathbf{x}), y)] \\
\hat{f}_{\mathcal{F}} &= \arg\min_{f \in \mathcal{F}} \hat{L}(f) \quad \text{(ERM model)} \\
\hat{f}_{\mathcal{F}}^T & \quad \text{(model produced by the algorithm at } T\text{'s iteration)}
\end{aligned}
$$

Decomposition of Learning Error

Excess risk: Optimization Error Estimation Error Approximation Error

$$L(\hat{f}_{\mathcal{F}}^{T}) - L(f^{*}) = \left(L(\hat{f}_{\mathcal{F}}^{T}) - L(\hat{f}_{\mathcal{F}})\right) + \left(L(\hat{f}_{\mathcal{F}}) - L(f_{\mathcal{F}})\right) + \left(L(f_{\mathcal{F}}) - L(f^{*})\right)$$



Guarantees for Three Errors

- Optimization error
  - Convergence rate of optimization algorithm
  - $L(\hat{f}_{\mathcal{F}}^{T}) - L(\hat{f}_{\mathcal{F}}) \leq \epsilon(Alg, \mathcal{F}, N, T)$
- Estimation / generalization error:
  - Upper bound in terms of capacity
  - $L(\hat{f}_{\mathcal{F}}) - L(f_{\mathcal{F}}) \leq 2 \sup_{f \in \mathcal{F}} |\hat{L}(f) - L(f)| \leq \epsilon(Cap(\mathcal{F}), N)$
- Approximation error
  - Cannot be controllable in general
  - Universal approximation theorem of neural networks

Cross Validation

- Hold-out cross validation: split training set $\mathcal{D}$ into training set and validation set.
  - waste training data!
- k-fold cross validation
  - commonly used choice: $k = 10$
  - If data is really scarce, we may set $k = N$, which is leave-one-out cross validation.
  - bias-variance tradeoff
- Note that test set is never used in cross validation.

Feature Selection

- Given labeled data, we compute some scores that measures how informative each feature is about the class label.
- Ranking criteria:
  - mutual information
  - Bayes error
  - redundancy
- Feature select schemes:
  - filter: direct feature ranking
  - wrapper: determine the features based on performance under the learning algorithms to be used.
  - simultaneous learning and feature selection. E.g., lasso, Bayesian feature selection, etc.

Frequentist vs. Bayesian

- Frequentist: The parameters are constant-valued but unknown.
- Bayesian: The parameters are random variables whose values are unknown. We would specify prior distribution to express our "prior beliefs" about the parameters.
- In practice, Bayesian MAP estimate is less susceptible to overfitting than the ML estimate of the parameters, which also automatically determines model complexity using training data alone.
- An example: for text classification with $D \gg N$, Bayesian logistic regression turns out to be an effective algorithm.

Bayesian Model Selection

- Bayesian model selection is used when there exists prior knowledge about the appropriate class of approximating functions, represented as a prior distribution over models, $p(\text{model})$.
- Posterior distribution over models given the data:

$$p(\text{model}|\text{data}) = \frac{p(\text{data}|\text{model})p(\text{model})}{p(\text{data})}$$

- From the posterior distribution, we may:
  - choose the model with the highest posterior probability, or
  - choose multiple models with high posterior probabilities, or
  - use all models weighted by their posterior probabilities.
- Regularization may be seen as a Bayesian approach in which the prior favors simpler models.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