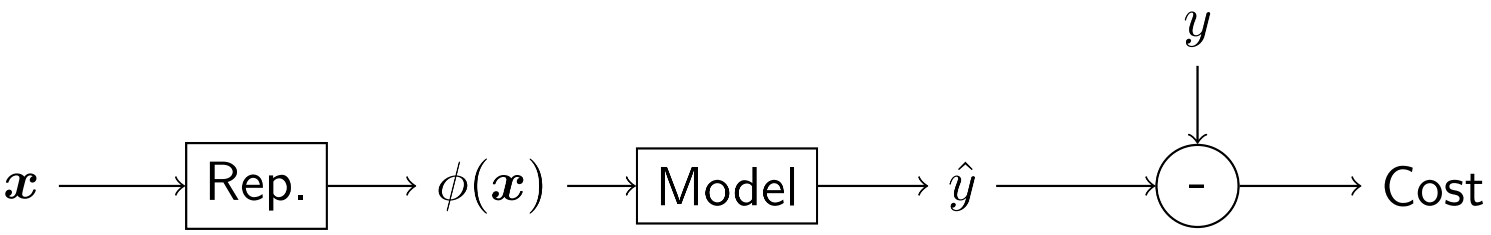
Chapter 5

Machine Learning Basics

Learning Algorithms

- (Mitchell, 1997) A computer program is said to learn from *experience* E with respect to some class of *tasks* T and *performance measure* P, if its performance at tasks in T, as measured by P, improves with experience E

- Example: Linear Regression



  - Task T: To predict y from $\boldsymbol{x}$ by outputting

$$\hat{y} = \boldsymbol{w}^T \phi(\boldsymbol{x}) = \phi(\boldsymbol{x})^T \boldsymbol{w}$$

  - Experience E: To learn $\boldsymbol{w}$ by minimizing, over a training set

$(\boldsymbol{X}^{(\text{train})}, \boldsymbol{y}^{(\text{train})})$,

$$\text{MSE}^{(\text{train})} = \frac{1}{m^{(\text{train})}} \|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2$$

where

$$\hat{\boldsymbol{y}}^{(\text{train})} = \boldsymbol{\Phi}^{(\text{train})}\boldsymbol{w}, \quad \boldsymbol{\Phi}^{(\text{train})} = \begin{bmatrix} \phi(\boldsymbol{x}_0^{(\text{train})})^T \\ \phi(\boldsymbol{x}_1^{(\text{train})})^T \\ \vdots \\ \phi(\boldsymbol{x}_{m-1}^{(\text{train})})^T \end{bmatrix}$$

$$\boldsymbol{y}^{(\text{train})} = (y_0^{(\text{train})}, y_1^{(\text{train})}, \ldots, y_{m-1}^{(\text{train})})$$

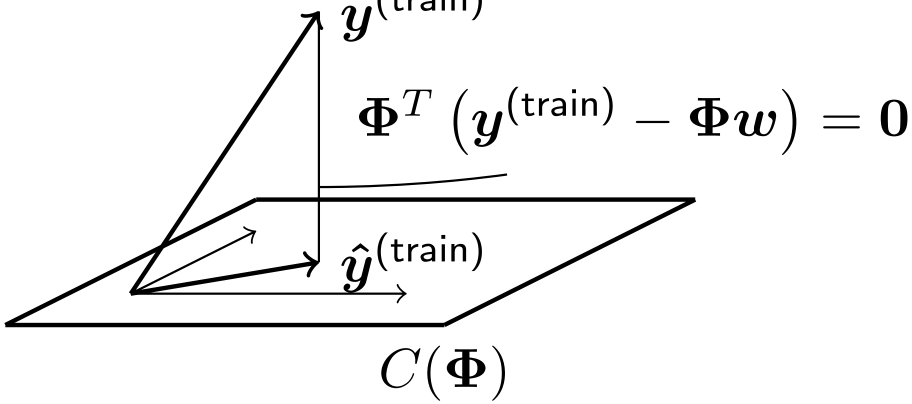
– Performance P: To measure mean squared error on a test set $(\boldsymbol{X}^{(\text{test})}, \boldsymbol{y}^{(\text{test})})$, i.e.,

$$\text{MSE}^{(\text{test})} = \frac{1}{m^{(\text{test})}} \|\hat{\boldsymbol{y}}^{(\text{test})} - \boldsymbol{y}^{(\text{test})}\|_2^2$$

- To minimize $\mathsf{MSE}_{\mathsf{train}}$, $\boldsymbol{w}$ can be solved by setting

$$\nabla_{\boldsymbol{w}} \mathsf{MSE}^{(\mathsf{train})} = \mathbf{0}$$

- A geometrical view is to solve $\hat{\boldsymbol{y}}^{(\mathsf{train})}$ as the projection of $\boldsymbol{y}^{(\mathsf{train})}$ onto the column space of $\boldsymbol{\Phi}^{(\mathsf{train})}$


$\boldsymbol{y}^{(\mathsf{train})}$
$\boldsymbol{\Phi}^T \left(\boldsymbol{y}^{(\mathsf{train})} - \boldsymbol{\Phi}\boldsymbol{w}\right) = \mathbf{0}$
$\hat{\boldsymbol{y}}^{(\mathsf{train})}$
$C(\boldsymbol{\Phi})$

- We then have

$$\boldsymbol{w} = \left(\boldsymbol{\Phi}^{(\mathsf{train})T} \boldsymbol{\Phi}^{(\mathsf{train})}\right)^{-1} \boldsymbol{\Phi}^{(\mathsf{train})T} \boldsymbol{y}^{\mathsf{train}}$$

- The present model can be extended to include a bias term b

$$\hat{y} = \boldsymbol{w}^T \phi(\boldsymbol{x}) + b = \tilde{\boldsymbol{w}}^T \tilde{\phi}(\boldsymbol{x}),$$

with

$$\tilde{\boldsymbol{w}} = \begin{bmatrix} \boldsymbol{w} \\ b \end{bmatrix}, \ \tilde{\phi}(\boldsymbol{x}) = \begin{bmatrix} \phi(\boldsymbol{x}) \\ 1 \end{bmatrix}$$

- Prediction with a polynominal of degree 2:

$$\hat{y} = w_2 x^2 + w_1 x^1 + b = \tilde{\boldsymbol{w}}^T \tilde{\phi}(x),$$

where

$$\tilde{\boldsymbol{w}} = \begin{bmatrix} w_2 \\ w_1 \\ b \end{bmatrix}, \ \tilde{\phi}(x) = \begin{bmatrix} \phi_2(x) \\ \phi_1(x) \\ 1 \end{bmatrix} = \begin{bmatrix} x^2 \\ x^1 \\ 1 \end{bmatrix}$$

Generalization

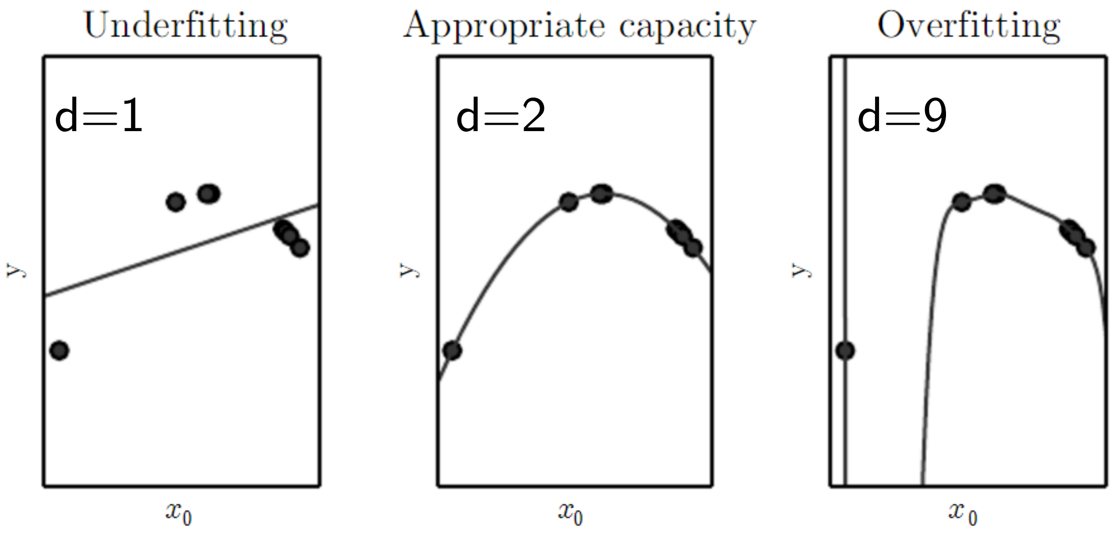
- The model's ability to perform well on *new, previously unseen* inputs
- Generalization error is defined to be the *expected value of the error* on a *new input* and is typically estimated by measuring the performance on a *test set* collected separately from the *training set*
- Examples $(\boldsymbol{x}, y)$ in the training and test sets are assumed to be drawn independently from the same distribution, $p_{\text{data}}(\boldsymbol{x}, y)$
- **Bayes error:** Minimum generalization error achieved by an oracle model having knowledge of $p_{\text{data}}(\boldsymbol{x}, y)$
- E.g.: if $y = \boldsymbol{w}^T \phi(\boldsymbol{x}) + \varepsilon$ and ε is Gaussian noise independent of $\boldsymbol{x}$, Bayes error $=$ Var(ε) with MSE measure

Training Error and Test Error

- (Pitfall) At first glance, the expected test error should be the same as the expected training error for a given model, because the data in these sets are drawn from the same distribution
- In practice, we sample the training set, use it to train the model, and then sample the test set to measure test error
- Generally, test error $\geq$ training error

Underfitting vs. Overfitting

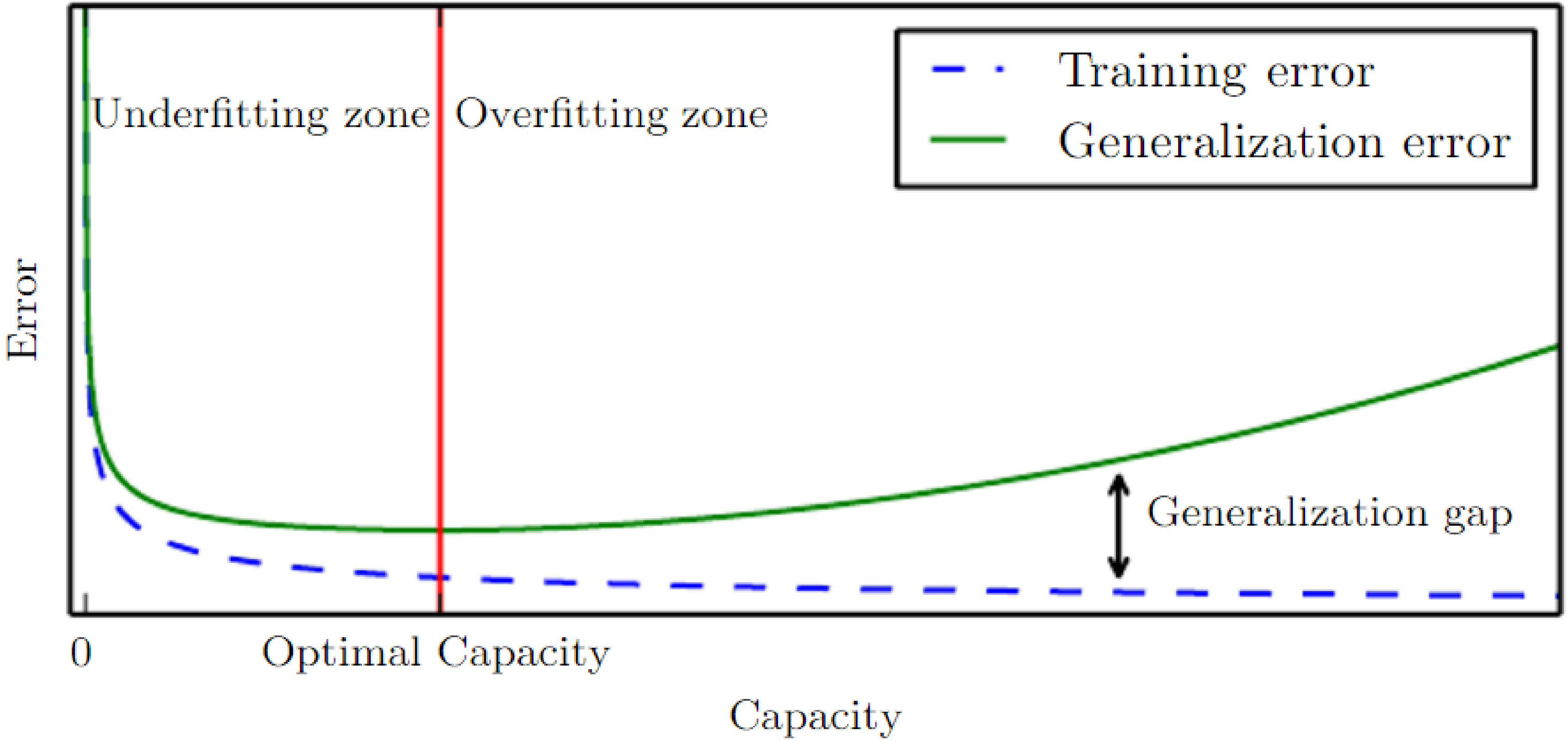
- Two objectives to achieve in designing a model
  1. Make training error small to avoid **underfitting**
  2. Make gap between training and test error small to avoid **overfitting**
- Trade-off can be made by altering the *model capacity*, which refers broadly to a model's ability to fit a wide variety of functions
- Example: Fitting a polynomial model to quadratic data



$$\hat{y} = \sum_{i=1}^{d} w_i x_0^i + b$$

Capacity and Error

Typical relationship between capacity and error

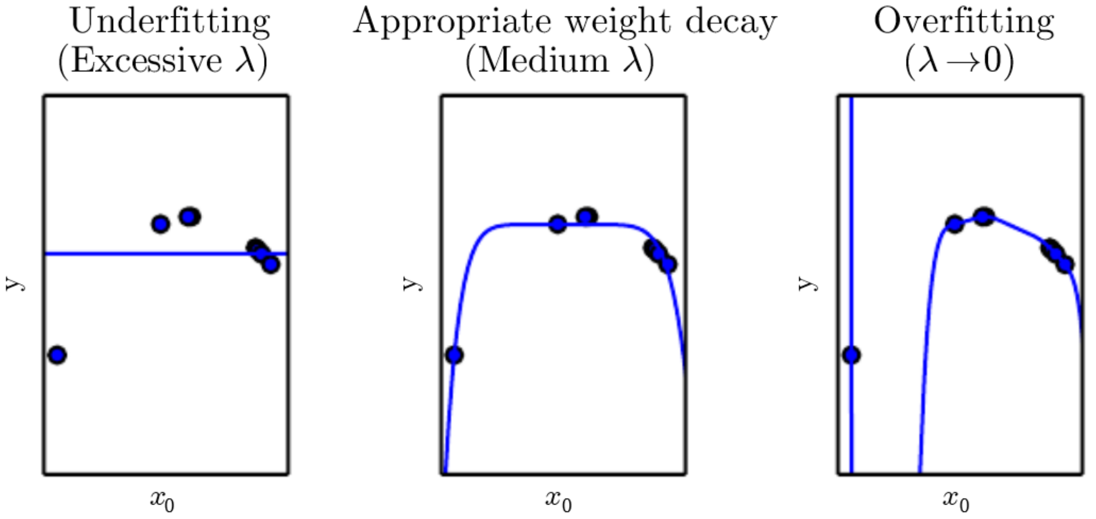


Regularization

- Modification made to the learning algorithm to reduce generalization error (usually at the cost of higher training error)
- Example: To include *weight decay* in the training criterion

$$J(\boldsymbol{w}) = \text{MSE}^{(\text{train})} + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

where λ controls preference for small $\boldsymbol{w}$ and is determined a priori



A degree-9 polynomial model fitted to quadratic data

Estimators

- **Point estimation:** To provide a single estimate of some quantity from observing independent and identically distributed (i.i.d.) samples
  - Consider m i.i.d samples $\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$ drawn from a Bernoulli distribution with mean θ

$$P(x^{(i)};\theta) = \theta^{x^{(i)}}(1-\theta)^{1-x^{(i)}},\ x^{(i)} = \{1,0\}$$

  - The *sample mean* can be used to give a point estimate of θ

$$\hat{\theta}_m = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$$

- A point estimator $\hat{\boldsymbol{\theta}}_m$ of a parameter $\boldsymbol{\theta}$ is any function of the observed samples $\{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)}\}$

$$\hat{\boldsymbol{\theta}}_m = g(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)})$$

- $\boldsymbol{\theta}$ is fixed but unknown from the **frequentist** viewpoint
- $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)}$ are seen samples of a random variable
- As a result, $\hat{\boldsymbol{\theta}}_m$ is a random variable

Bias

- The bias of the estimator $\hat{\boldsymbol{\theta}}_m$ is defined as

$$\text{bias}(\hat{\boldsymbol{\theta}}_m) = E(\hat{\boldsymbol{\theta}}_m) - \boldsymbol{\theta},$$

  where the expectation $E(\cdot)$ is taken w.r.t. $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)}$

  – $\hat{\boldsymbol{\theta}}_m$ is *unbiased* if bias($\hat{\boldsymbol{\theta}}_m$)=0

  – $\hat{\boldsymbol{\theta}}_m$ is *asymptotically unbiased* if $\lim_{m\to\infty}$ bias$(\hat{\boldsymbol{\theta}}_m) = 0$

- In the Bernoulli example, the sample mean is an unbiased estimator

$$E\left[\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right] = \frac{1}{m}\sum_{i=1}^{m} E\left[x^{(i)}\right] = \theta$$

Consistency

- An estimator $\hat{\boldsymbol{\theta}}_m$ is said to be consistent *in probability* if

$$\lim_{m\to\infty} P\left(\left|\hat{\boldsymbol{\theta}}_m - \boldsymbol{\theta}\right| > \varepsilon\right) = 0, \ \varepsilon > 0$$

- Consistency ensures that the bias of the estimator diminishes as the number of data samples grows

- In the Bernoulli example, the sample mean is consistent
  - Chebyshev's inequality

$$P(|X - \mu_X| > \varepsilon) \leq \frac{\sigma_x^2}{\varepsilon^2}$$

  - $\hat{\theta}_m$ has mean θ, variance $\theta(1-\theta)/m$

$$P(|\hat{\theta}_m - \theta| > \varepsilon) \leq \frac{\theta(1-\theta)}{m\varepsilon^2} \Rightarrow \lim_{m\to\infty} P(|\hat{\theta}_m - \theta| > \varepsilon) = 0$$

Estimators for Gaussian Distribution

- Gaussian probability density function

$$\mathcal{N}(x^{(i)};\mu,\sigma^2)=\frac{1}{\sqrt{2\pi\sigma^2}}\mathsf{exp}\left(-\frac{1}{2}\frac{(x^{(i)}-\mu)^2}{\sigma^2}\right)$$

- Sample mean (unbiased)

$$\hat{\mu}_m=\frac{1}{m}\sum_{i=1}^{m}x^{(i)}$$

- Sample variance (asymptotically unbiased)

$$\hat{\sigma}_m^2=\frac{1}{m}\sum_{i=1}^{m}\left(x^{(i)}-\hat{\mu}_m\right)^2$$

  - It can be shown that $E[\hat{\sigma}_m^2]=(m-1)\sigma^2/m$
  - Unbiased sample variance $\tilde{\sigma}_m^2=m\hat{\sigma}_m^2/(m-1)$

Variance of the Estimator[†]

- Variance of the estimator indicates how much the estimator varies as a function of the samples; and its squared root is called standard error
- Example: Standard error of the sample mean $\hat{\mu}_m$

$$\mathsf{SE}(\hat{\mu}_m) = \sqrt{\mathsf{Var}\left[\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right]} = \frac{\sigma}{\sqrt{m}}$$

where σ is usually estimated by $\sqrt{\tilde{\sigma}_m^2}$

- By the central limit theorem,

$$\frac{\hat{\mu}_m - \mu}{\mathsf{SE}(\hat{\mu}_m)} \sim \mathcal{N}(0,1)$$

- The 95 percent confidence interval can thus be derived as

$$(\hat{\mu}_m - 1.96\mathsf{SE}(\hat{\mu}_m), \hat{\mu}_m + 1.96\mathsf{SE}(\hat{\mu}_m))$$

- In experiments, it is common to say algorithm A performs better than B if its 95 percent upper bound of the test error is smaller than the lower bound of B's test error

Maximum Likelihood (ML) Estimation

- Consider examples $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)}$ drawn independently from a distribution $p_{\mathsf{model}}(\boldsymbol{x}; \boldsymbol{\theta})$, with parameter $\boldsymbol{\theta}$ being fixed but unknown
- The maximum likelihood estimator $\boldsymbol{\theta}_{\mathsf{ML}}$ for $\boldsymbol{\theta}$ is defined as

$$\begin{aligned} \boldsymbol{\theta}_{\mathsf{ML}} &= \arg\max_{\boldsymbol{\theta}} p_{\mathsf{model}}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)}; \boldsymbol{\theta}) \\ &= \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{m} p_{\mathsf{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}) \\ &= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log p_{\mathsf{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}) \end{aligned}$$

  where $\sum_{i=1}^{m} \log p_{\mathsf{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$ is the *log-likelihood function* of $\boldsymbol{\theta}$

- The sum over examples can be written as expectation w.r.t. the empirical data distribution $\hat{p}_{\text{data}}$

$$\boldsymbol{\theta}_{\text{ML}} = \arg\max_{\boldsymbol{\theta}} E_{\boldsymbol{x}\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x};\boldsymbol{\theta})$$

- Maximizing the log-likelihood amounts to minimizing the dissimilarity between the empirical data distribution $\hat{p}_{\text{data}}$ (defined by the training set) and the model distribution p_{model} in terms of KL divergence:

$$D_{KL}(\hat{p}_{\text{data}}\|p_{\text{model}}) = E_{\boldsymbol{x}\sim\hat{p}_{\text{data}}}[\log \hat{p}_{\text{data}}(\boldsymbol{x}) - \log p_{\text{model}}(\boldsymbol{x};\boldsymbol{\theta})]$$

- Remarks
  - In information theory, $D_{KL}(\hat{p}_{\text{data}}\|p_{\text{model}})$ denotes the extra amount of information (in bits when using $\log_2$ base) needed to send a message $\boldsymbol{x}$ drawn from $\hat{p}_{\text{data}}$ with a code optimized for messages drawn from p_{model}
  - The *cross-entropy* $H(\hat{p}_{\text{data}}, p_{\text{model}})$ between $\hat{p}_{\text{data}}$ and p_{model} is defined as

$$-E_{\boldsymbol{x}\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x};\boldsymbol{\theta})$$

- It is easy to show that

$$-E_{\boldsymbol{x}\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x};\boldsymbol{\theta}) = H(\hat{p}_{\text{data}}) + D_{KL}(\hat{p}_{\text{data}}\|p_{\text{model}})$$

- Minimizing the cross-entropy $H(\hat{p}_{\text{data}}, p_{\text{model}})$ is equivalent to maximizing the log-likelihood function $E_{\boldsymbol{x}\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x};\boldsymbol{\theta})$ and thus minimizing the $D_{KL}(\hat{p}_{\text{data}}\|p_{\text{model}})$

Conditional Log-Likelihood Estimation

- The ML estimator generalized to learn a conditional probability $p_{\text{model}}(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})$ in order to predict $\boldsymbol{y}$ given $\boldsymbol{x}$

$$\begin{aligned}\boldsymbol{\theta}_{\text{ML}} &= \arg\max_{\boldsymbol{\theta}} p_{\text{model}}(\boldsymbol{Y}|\boldsymbol{X};\boldsymbol{\theta}) \\ &= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log p_{\text{model}}(\boldsymbol{y}^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{\theta}) \\ &= \arg\max_{\boldsymbol{\theta}} E_{\boldsymbol{x},\boldsymbol{y}\sim\hat{p}_{\text{data}}(\boldsymbol{x},\boldsymbol{y})} \log p_{\text{model}}(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})\end{aligned}$$

- Example: Linear Regression

$$y = \hat{y}(\boldsymbol{x};\boldsymbol{w}) + \varepsilon = \boldsymbol{w}^T\phi(\boldsymbol{x}) + \varepsilon$$

where $\varepsilon \sim \mathcal{N}(0,\sigma^2)$ is independent of $\boldsymbol{x}$

  - It can be shown that $p(y|\boldsymbol{x};\boldsymbol{w}) = \mathcal{N}(y;\hat{y}(\boldsymbol{x};\boldsymbol{w}),\sigma^2)$
  - The conditional log-likelihood of $p_{\text{model}}(\boldsymbol{Y}|\boldsymbol{X};\boldsymbol{w})$ is given by

$$\sum_{i=1}^{m} \log p(y^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{w}) = -m\log\sigma - \frac{m}{2}\log(2\pi) - \sum_{i=1}^{m}\frac{(\hat{y}^{(i)}-y^{(i)})^2}{2\sigma^2}$$

- Maximizing the log-likelihood w.r.t. $\boldsymbol{w}$ leads to the same problem of minimizing

$$\text{MSE}^{(\text{train})} = \frac{1}{m^{(\text{train})}}\|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2$$

- Therefore, the data model $y = \hat{y}(\boldsymbol{x};\boldsymbol{w}) + \varepsilon$ provides an alternative view of the linear regression problem

Bayesian Statistics

- Assume the true parameter $\boldsymbol{\theta}$ is a random variable governed by a prior probability distribution $p(\boldsymbol{\theta})$
- The goal is to infer the posterior distribution $p(\boldsymbol{\theta}|\boldsymbol{X})$ of $\boldsymbol{\theta}$ by combining the prior $p(\boldsymbol{\theta})$ and the data likelihood $p(\boldsymbol{X}|\boldsymbol{\theta})$ via Bayes' rule:

$$p(\boldsymbol{\theta}|\boldsymbol{X}) = \frac{p(\boldsymbol{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\boldsymbol{X})}$$

- Example: Linear Regression

$$y = \hat{y}(\boldsymbol{x}; \boldsymbol{w}) + \varepsilon = \boldsymbol{w}^T \phi(\boldsymbol{x}) + \varepsilon$$

  - Again, $p(y|\boldsymbol{x}, \boldsymbol{w}) = \mathcal{N}(y; \hat{y}(\boldsymbol{x}; \boldsymbol{w}), \sigma^2)$, where presently $\sigma^2 = 1$
  - Assume $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu_0}, \boldsymbol{\Lambda_0})$
  - Consider $\boldsymbol{x}$ to be deterministic data

– The posterior distribution $p(\boldsymbol{w}|\boldsymbol{X}^{(\text{train})}, \boldsymbol{y}^{(\text{train})})$ is given by

$$
\begin{aligned}
& p(\boldsymbol{w}|\boldsymbol{X}^{(\text{train})}, \boldsymbol{y}^{(\text{train})}) \\
& \propto p(\boldsymbol{w})p(\boldsymbol{y}^{(\text{train})}|\boldsymbol{X}^{(\text{train})}, \boldsymbol{w}) \\
& \propto \text{exp}(-\frac{1}{2}(\boldsymbol{w}-\boldsymbol{u}_0)^T\boldsymbol{\Lambda}_0^{-1}(\boldsymbol{w}-\boldsymbol{u}_0))\text{exp}(-\frac{1}{2}(\boldsymbol{y}-\boldsymbol{\Phi}\boldsymbol{w})^T(\boldsymbol{y}-\boldsymbol{\Phi}\boldsymbol{w})) \\
& \propto \text{exp}(-\frac{1}{2}(\boldsymbol{w}-\boldsymbol{u}_m)^T\boldsymbol{\Lambda}_m^{-1}(\boldsymbol{w}-\boldsymbol{u}_m)) \\
& = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}_m, \boldsymbol{\Lambda}_m)
\end{aligned}
$$

where

$$
\begin{aligned}
\boldsymbol{\Phi} &= \boldsymbol{\Phi}^{(\text{train})} \\
\boldsymbol{\Lambda}_m &= (\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \boldsymbol{\Lambda}_0^{-1})^{-1} \\
\boldsymbol{u}_m &= \boldsymbol{\Lambda}_m(\boldsymbol{\Phi}^T\boldsymbol{y}^{(\text{train})} + \boldsymbol{\Lambda}_0^{-1}\boldsymbol{u}_0)
\end{aligned}
$$

– When $\boldsymbol{\mu}_0 = \boldsymbol{0}$ and $\boldsymbol{\Lambda}_0 = \frac{1}{\lambda}\boldsymbol{I}$, $\boldsymbol{\mu}_m$ leads to the same solution as minimizing

$$J(\boldsymbol{w}) = \mathsf{MSE}^{(\mathsf{train})} + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

- Given $p(\boldsymbol{w}|\boldsymbol{X}^{(\mathsf{train})}, \boldsymbol{y}^{(\mathsf{train})})$, one can infer the probability distribution of $y^{(\mathsf{new})}$ at unseen $\boldsymbol{x}^{(\mathsf{new})}$ by

$$\begin{aligned} & p(y^{(\mathsf{new})}|\boldsymbol{x}^{(\mathsf{new})}, \boldsymbol{X}^{(\mathsf{train})}, \boldsymbol{y}^{(\mathsf{train})}) \\ &= \int p(y^{(\mathsf{new})}, \boldsymbol{w}|\boldsymbol{x}^{(\mathsf{new})}, \boldsymbol{X}^{(\mathsf{train})}, \boldsymbol{y}^{(\mathsf{train})}) d\boldsymbol{w} \\ &= \int p(\boldsymbol{w}|\boldsymbol{X}^{(\mathsf{train})}, \boldsymbol{y}^{(\mathsf{train})}) p(y^{(\mathsf{new})}|\boldsymbol{x}^{(\mathsf{new})}, \boldsymbol{w}) d\boldsymbol{w} \\ &= \int \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}_m, \boldsymbol{\Lambda}_m) \mathcal{N}(y^{(\mathsf{new})}; \hat{y}(\boldsymbol{x}^{(\mathsf{new})}; \boldsymbol{w}), 1) d\boldsymbol{w} \end{aligned}$$

- Equivalently, this is to ask about the distribution of

$$y^{(\mathsf{new})} = \hat{y}(\boldsymbol{x}^{(\mathsf{new})}; \boldsymbol{w}) + \varepsilon = \boldsymbol{w}^T \phi(\boldsymbol{x}^{(\mathsf{new})}) + \varepsilon$$

given $(\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})})$, with

$$p(\boldsymbol{w}|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}_m, \boldsymbol{\Lambda}_m)$$

$$p(\varepsilon|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}) = \mathcal{N}(\varepsilon; 0, 1)$$

and $\boldsymbol{w}$, ε being conditionally independent

$$\begin{aligned} & p(\boldsymbol{w}, \varepsilon|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}) \\ & = p(\boldsymbol{w}|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}) p(\varepsilon|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}) \end{aligned}$$

- We further recognize that

1. $\boldsymbol{w}^T \phi(\boldsymbol{x}^{(\text{new})})|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}$ is a Gaussian

$$\begin{aligned} & \boldsymbol{w}^T \phi(\boldsymbol{x}^{(\text{new})})|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})} \\ & \sim \mathcal{N}(\boldsymbol{\mu}_m^T \phi(\boldsymbol{x}^{(\text{new})}), \phi(\boldsymbol{x}^{(\text{new})})^T \boldsymbol{\Lambda}_m \phi(\boldsymbol{x}^{(\text{new})})) \end{aligned}$$

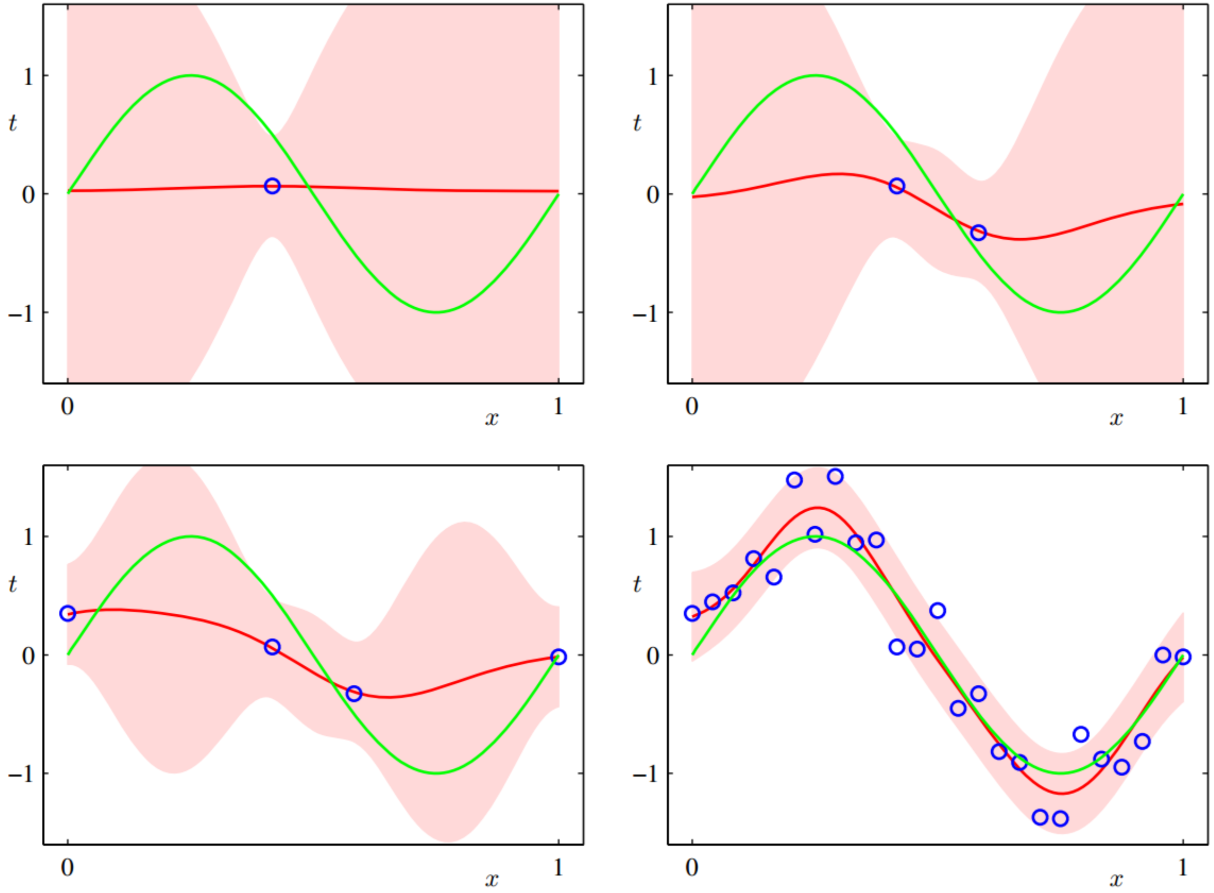
2. $\boldsymbol{w}^T \phi(\boldsymbol{x}^{(\text{new})}) + \varepsilon|\boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})}$ (sum of two conditionally

independent Gaussian's) is another Gaussian

$$\begin{aligned} &\boldsymbol{w}^T\phi(\boldsymbol{x}^{(\text{new})}) + \varepsilon | \boldsymbol{X}^{(\text{train})}, \boldsymbol{Y}^{(\text{train})} \\ &\sim \mathcal{N}(\boldsymbol{\mu}_m^T\phi(\boldsymbol{x}^{(\text{new})}), \phi(\boldsymbol{x}^{(\text{new})})^T\boldsymbol{\Lambda}_m\phi(\boldsymbol{x}^{(\text{new})}) + 1) \end{aligned}$$

- This concludes our evaluation for $p(y^{(\text{new})}|\boldsymbol{x}^{(\text{new})}, \boldsymbol{X}^{(\text{train})}, \boldsymbol{y}^{(\text{train})})$

Bayesian Statistics



Ground truth (Green); $\mu_{y^{(\text{new})}}$ (Red); Data (Blue); $\sigma_{y^{(\text{new})}}$ (Pink)

Maximum A Posteriori (MAP) Estimation

- The full Bayesian treatment may sometimes be intractable
- To offer a point estimate in the Bayesian framework, we usually choose

$$\begin{aligned}\boldsymbol{\theta}_{\text{MAP}} &= \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\boldsymbol{X}) \\ &= \arg\max_{\boldsymbol{\theta}} \frac{p(\boldsymbol{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\boldsymbol{X})} \\ &= \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\end{aligned}$$

- Many regularized estimation strategies (e.g. ML+weight decay) can be interpreted as making the MAP inference, if the regularization term (e.g. weight decay) admits an explanation of $\log p(\boldsymbol{\theta})$
- Example: Linear Regression

$$\boldsymbol{w}_{\text{MAP}} = \arg\max_{\boldsymbol{w}} p(\boldsymbol{w}|\boldsymbol{X}^{(\text{train})}, \boldsymbol{y}^{(\text{train})})$$

$$
\begin{aligned}
&= \arg\max_{\boldsymbol{w}} \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}_m, \boldsymbol{\Lambda}_m) \\
&= \boldsymbol{\mu}_m
\end{aligned}
$$

- We may then choose the prediction model to be

$$\hat{y}(\boldsymbol{x}^{(\mathsf{new})}; \boldsymbol{w}) = \boldsymbol{w}_{\mathsf{MAP}}^T \phi(\boldsymbol{x}^{(\mathsf{new})}) = \boldsymbol{\mu}_m^T \phi(\boldsymbol{x}^{(\mathsf{new})}),$$

which in the present case coincides with the mean of the posterior distribution $p(y^{(\mathsf{new})}|\boldsymbol{x}^{(\mathsf{new})}, \boldsymbol{X}^{(\mathsf{train})}, \boldsymbol{y}^{(\mathsf{train})})$

- From the earlier derivation and definitions,

$$\boldsymbol{\mu}_m = \boldsymbol{\Lambda}_m(\boldsymbol{\Phi}^T \boldsymbol{y}^{(\mathsf{train})} + \boldsymbol{\Lambda}_0^{-1} \boldsymbol{u}_0)$$

$$\boldsymbol{\Phi} = \begin{bmatrix} \phi(\boldsymbol{x}_0^{(\mathsf{train})})^T \\ \phi(\boldsymbol{x}_1^{(\mathsf{train})})^T \\ \vdots \\ \phi(\boldsymbol{x}_{m-1}^{(\mathsf{train})})^T \end{bmatrix}, \; \boldsymbol{y}^{(\mathsf{train})} = \begin{bmatrix} y_0^{(\mathsf{train})} \\ y_1^{(\mathsf{train})} \\ \vdots \\ y_{m-1}^{(\mathsf{train})} \end{bmatrix}$$

- Assuming $\boldsymbol{\mu}_0 = 0$, we have

$$\begin{aligned}\hat{y}(\boldsymbol{x}^{(\text{new})};\boldsymbol{w}) &= \phi(\boldsymbol{x}^{(\text{new})})^T \boldsymbol{\Lambda}_m \boldsymbol{\Phi}^T \boldsymbol{y}^{(\text{train})} \\ &= \sum_{i=0}^{m-1} \underbrace{\phi(\boldsymbol{x}^{(\text{new})})^T \boldsymbol{\Lambda}_m \phi(\boldsymbol{x}_i^{(\text{train})})} y_i^{(\text{train})} \\ &= \sum_{i=0}^{m-1} \underbrace{k(\boldsymbol{x}^{(\text{new})}, \boldsymbol{x}_i^{(\text{train})})}_{\text{Kernel}} y_i^{(\text{train})}\end{aligned}$$

where

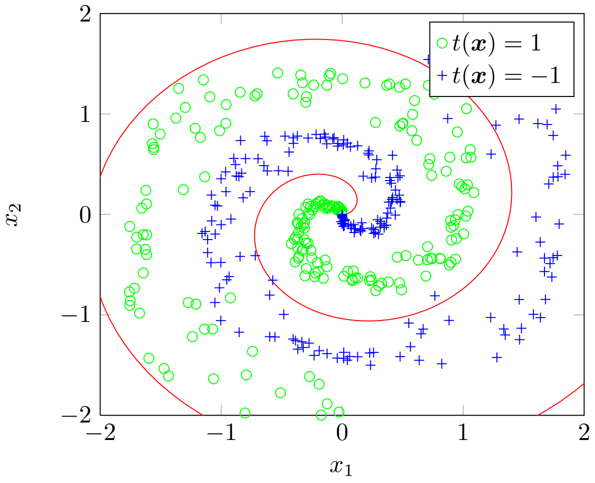
$$k(\boldsymbol{x}^{(\text{new})}, \boldsymbol{x}_i^{(\text{train})}) = \phi(\boldsymbol{x}^{(\text{new})})^T \boldsymbol{\Lambda}_m \phi(\boldsymbol{x}_i^{(\text{train})})$$

- It is seen that the prediction $\hat{y}(\boldsymbol{x}^{(\text{new})};\boldsymbol{w})$ is a weighted combination of the training data $y_i^{(\text{train})}$ with weights determined by the kernel function $k(\cdot)$ measuring a certain type of distance between $\boldsymbol{x}^{(\text{new})}$ and $\boldsymbol{x}_i^{(\text{train})}$

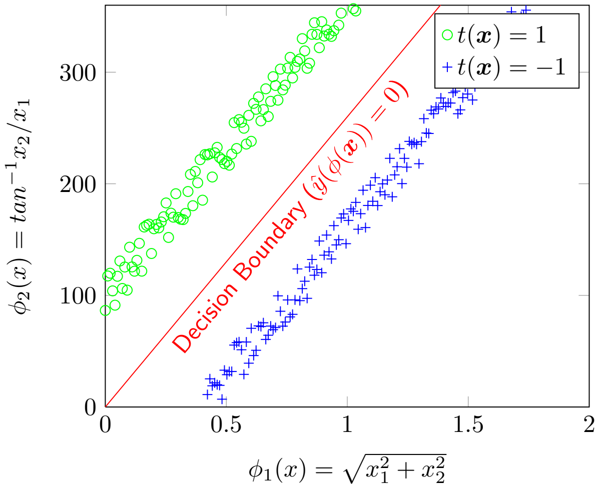
Support Vector Machines (SVM)†

- One of the most influential approaches to supervised learning
- **Idea:** To find a hyperplane (in feature space) for classifying linearly separable training data according to the sign of $\hat{y}(\phi(\boldsymbol{x}))$

$$\hat{y}(\phi(\boldsymbol{x})) = \boldsymbol{w}^T \phi(\boldsymbol{x}) + b$$



raw data domain



feature domain

- The hyperplane, known as the decision boundary, is defined by

$$\hat{y}(\phi(\boldsymbol{x})) = \boldsymbol{w}^T\phi(\boldsymbol{x}) + b = 0$$

- $\boldsymbol{w}$ is a vector orthogonal to every vector in the decision boundary
- Any point $\phi(\boldsymbol{x})$ to the decision boundary has a distance

$$\frac{|\hat{y}(\phi(\boldsymbol{x}))|}{\|\boldsymbol{w}\|}$$

- **Maximum margin classifiers**: Maximizing the smallest distance between the decision boundary and any of the training samples $\phi(\boldsymbol{x}_n)$

$$\arg\max_{\boldsymbol{w},b}\min_n \frac{t_n\hat{y}(\phi(\boldsymbol{x}_n))}{\|\boldsymbol{w}\|} = \arg\max_{\boldsymbol{w},b}\left\{\frac{1}{\|\boldsymbol{w}\|}\min_n[t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n)+b)]\right\}$$

where $t_n \in \{-1, 1\}$ is the ground-truth label associated with $\phi(\boldsymbol{x}_n)$

- Noting that $\boldsymbol{w}, b$ can be scaled simultaneously $(\boldsymbol{w} \rightarrow \kappa\boldsymbol{w}, b \rightarrow \kappa b)$ without changing the resulting distance, we can choose a κ such that

$t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n)+b)=1$ for the closest point $\phi(\boldsymbol{x}_n)$ to the boundary

- This allows us to reformulate the problem as a *constrained optimization problem*

$$\min \frac{1}{2}\|\boldsymbol{w}\|_2^2, \text{ subject to}$$

$$t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n)+b)\geq 1, \forall n$$

- Using the method of Lagrange multipliers, which will be introduced next, the solution for $\hat{y}(\phi(\boldsymbol{x}))$ can be solved as

$$\hat{y}(\phi(\boldsymbol{x}))=\sum_{i=1}^{N} a_n t_n \underbrace{\phi(\boldsymbol{x}_n)^T\phi(\boldsymbol{x})} + b = \sum_{i=1}^{N} a_n t_n \underbrace{k(\boldsymbol{x}_n,\boldsymbol{x})}_{\text{Kernel}} + b$$

where $a_n \geq 0, \forall n$ and most of them are zero

- *Support vectors* refer to those $\phi(\boldsymbol{x}_n)$'s whose $a_n \neq 0$

Constrained Optimization[†]

- To find the maximal/minimal value of $f(\boldsymbol{x})$ for $\boldsymbol{x}$ (known as feasible points) in some set $\mathbb{S}$, e.g.

$$\arg\min_{\boldsymbol{x}} f(\boldsymbol{x}),\ \text{subject to}$$
$$g^{(i)}(x) = 0,\ i = 1, \ldots, m$$
$$h^{(j)}(x) \le 0,\ j = 1, \ldots, n$$

where $\mathbb{S} = \{\boldsymbol{x} | \forall i, g^{(i)}(x) = 0,\ \forall j, h^{(j)} \le 0\}$ are defined by m *equality constraints* and n *inequality constraints*

- The **Karush-Kuhn-Tucker (KKT)** approach obtains a solution by solving the unconstrained optimization of the Lagrangian function:

$$\min_{\boldsymbol{x}} \max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \ge \boldsymbol{0}} L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha})$$

where

$$L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}) = f(\boldsymbol{x}) + \sum_{i=1}^{m} \lambda_i g^{(i)}(\boldsymbol{x}) + \sum_{j=1}^{n} \alpha_j h^{(j)}(\boldsymbol{x})$$

and $\boldsymbol{\lambda}$ and $\boldsymbol{\alpha}$ are termed Lagrange multipliers

- The optimal solution satisfies (necessary conditions)
  1. $\nabla L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}) = \mathbf{0}$
  2. All constraints on $\boldsymbol{x}$ and Lagrange multipliers are met
  3. Complementary slackness: $\boldsymbol{\alpha} \odot \boldsymbol{h}(\boldsymbol{x}) = \mathbf{0}$, i.e. $\alpha_j = 0$ for $h^{(j)}(\boldsymbol{x}) < 0$ (inactive) and $\alpha_j \geq 0$ for $h^{(j)}(\boldsymbol{x}) = 0$ (active)
- It is easy to see that when any constraint is violated,

$$\max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq \mathbf{0}} L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}) = \infty,$$

which excludes infeasible points from being considered

- On the other hand, when the constraints are all satisfied,

$$\max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha},\boldsymbol{\alpha}\geq\mathbf{0}} L(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\alpha}) = f(\boldsymbol{x}),$$

which ensures the optimum within feasible points is unchanged

- Example: To solve $\boldsymbol{w}, b$

$$\min \frac{1}{2}\|\boldsymbol{w}\|_2^2, \text{ subject to}$$

$$t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n)+b) \geq 1, \forall n$$

- We set to zero the gradient w.r.t.

$$L(\boldsymbol{w},b,\boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{w}\|_2^2 + \sum_{j=1}^{n}\alpha_j(1-t_j(\boldsymbol{w}^T\phi(\boldsymbol{x}_j)+b))$$

and arrive at

$$\nabla_{\boldsymbol{w}} L(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \mathbf{0} \Rightarrow \boldsymbol{w} = \sum_{j=1}^{n} \alpha_j t_j \phi(\boldsymbol{x}_j)$$

$$\nabla_b L(\boldsymbol{w}, b, \boldsymbol{\alpha}) = 0 \Rightarrow \sum_{j=1}^{n} \alpha_j t_j = 0$$

- At this point, we already have the form of the optimal $\boldsymbol{w}$
- To solve for $\boldsymbol{\alpha}$, we can substitute this $\boldsymbol{w}$ back to the Lagrangian

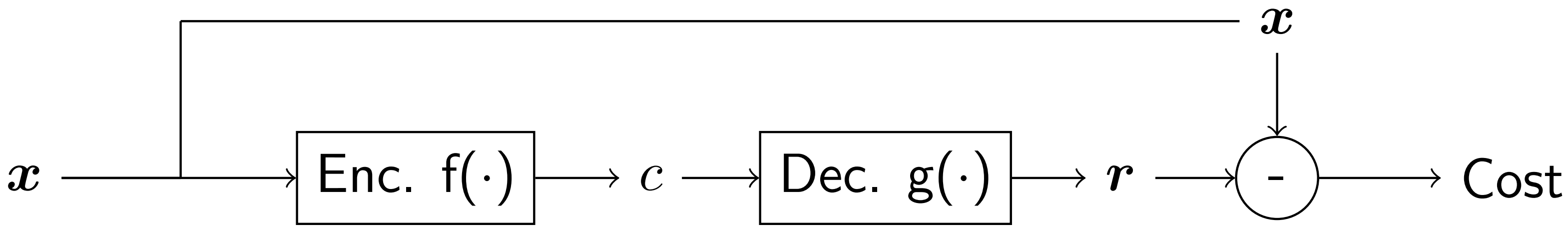
$$\max_{\boldsymbol{\alpha}} \sum_{j=1}^{n} \alpha_j - \frac{1}{2} \sum_{p=1}^{m} \sum_{q=1}^{m} \alpha_p \alpha_q t_p t_q \phi(\boldsymbol{x}_p)^T \phi(\boldsymbol{x}_q), \text{ s.t.}$$

$$\alpha_i \geq 0, \forall i \text{ and } \sum_{j=1}^{n} \alpha_j t_j = 0$$

- How to solve b? (To be continued)

Principle Component Analysis (PCA)

- An *unsupervised learning* algorithm that learns a data representation



$\boldsymbol{x}$ Enc. f(·) c Dec. g(·) $\boldsymbol{r}$ - Cost $\boldsymbol{x}$

  - Input: $\boldsymbol{x} \in \mathbb{R}^n$
  - Representation of input: $\boldsymbol{c} \in \mathbb{R}^l$
  - Decoder: $g(\boldsymbol{c}) = \boldsymbol{D}\boldsymbol{c}$ with $\boldsymbol{D}$ composed of orthonormal columns
  - Cost: $\|\boldsymbol{x} - g(\boldsymbol{c})\|_2^2$
  - Encoder has the form $f(\boldsymbol{x}) = \boldsymbol{D}^T\boldsymbol{x}$ when Cost is minimized

- Objective: Given training data $\boldsymbol{X}^{(\text{train})}$, we wish to find $\boldsymbol{D}$

$$\arg\min_{\boldsymbol{D}} \|\boldsymbol{X}^{(\text{train})} - \boldsymbol{X}^{(\text{train})}\boldsymbol{D}\boldsymbol{D}^T\|_F^2, \text{ s.t. } \boldsymbol{D}^T\boldsymbol{D} = \boldsymbol{I}$$

- Recall that

$$\boldsymbol{X}^{(\text{train})} = \begin{bmatrix} \boldsymbol{x}_0^{(\text{train})T} \\ \boldsymbol{x}_1^{(\text{train})T} \\ \vdots \\ \boldsymbol{x}_{m-1}^{(\text{train})T} \end{bmatrix}, \ \|\boldsymbol{A}\|_F^2 = \text{Tr}\{\boldsymbol{A}\boldsymbol{A}^T\} = \sum_{i,j} A_{i,j}^2$$

- By simple algebra, we have

$$\begin{aligned} &\|\boldsymbol{X}^{(\text{train})} - \boldsymbol{X}^{(\text{train})}\boldsymbol{D}\boldsymbol{D}^T\|_F^2 \\ &= \text{Tr}(\boldsymbol{X}^{(\text{train})}\boldsymbol{X}^{(\text{train})T}) - \text{Tr}(\boldsymbol{X}^{(\text{train})}\boldsymbol{D}\boldsymbol{D}^T\boldsymbol{X}^{(\text{train})T}) \end{aligned}$$

where the first term has nothing to do with $\boldsymbol{D}$

- The initial problem then simplifies to

$$\arg\max_{\boldsymbol{D}} \text{Tr}(\boldsymbol{X}^{(\text{train})}\boldsymbol{D}\boldsymbol{D}^T\boldsymbol{X}^{(\text{train})T}), \ \text{s.t.} \ \ \boldsymbol{D}^T\boldsymbol{D} = \boldsymbol{I}$$

- Observing that the Trace operator has the property

$$\mathsf{Tr}(\boldsymbol{ABC}) = \mathsf{Tr}(\boldsymbol{BCA}) = \mathsf{Tr}(\boldsymbol{CAB})$$

(as long as all matrix multiplications are allowed), we arrive at

$$\arg\max_{\boldsymbol{D}} \mathsf{Tr}(\boldsymbol{D}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})} \boldsymbol{D}), \text{ s.t. } \boldsymbol{D}^T \boldsymbol{D} = \boldsymbol{I}$$

- By a further application of Singular Value Decomposition to

$$\boldsymbol{X}^{(\text{train})}_{m\times n} = \boldsymbol{U}_{m\times m} \boldsymbol{\Sigma}_{m\times n} \boldsymbol{V}^T_{n\times n},$$

  - $\boldsymbol{U}$ is the eigenvector matrix of $\boldsymbol{X}^{(\text{train})}_{m\times n} \boldsymbol{X}^{(\text{train})T}_{m\times n}$ and satisfies

$$\boldsymbol{U}\boldsymbol{U}^T = \boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}_{m\times m}$$

  - $\boldsymbol{V}$ is the eigenvector matrix of $\boldsymbol{X}^{(\text{train})T}_{m\times n} \boldsymbol{X}^{(\text{train})}_{m\times n}$ and satisfies

$$\boldsymbol{V}\boldsymbol{V}^T = \boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}_{n\times n}$$

- $\boldsymbol{\Sigma}$ is the singular matrix given by

$$\left[\begin{array}{cccc:c} \sigma_1 & 0 & \dots & 0 & \\ 0 & \sigma_2 & \dots & 0 & \\ \vdots & \vdots & \ddots & 0 & \mathbf{0} \\ 0 & 0 & 0 & \sigma_r & \\ \hdashline \multicolumn{4}{c:}{\mathbf{0}} & \mathbf{0} \end{array}\right]_{m\times n}$$

- We see that the columns of $\boldsymbol{D}$ have an obvious choice of the l columns in $\boldsymbol{V}$ which corresponds to the largest l singular values

$$\arg\max_{\boldsymbol{D}} \mathsf{Tr}(\boldsymbol{D}^T\boldsymbol{V}\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{D}), \text{ s.t. } \boldsymbol{D}^T\boldsymbol{D} = \boldsymbol{I}$$

where

$$\boldsymbol{\Sigma}^T\boldsymbol{\Sigma} = \left[\begin{array}{cccc:c} \sigma_1^2 & 0 & \dots & 0 & \\ 0 & \sigma_2^2 & \dots & 0 & \\ \vdots & \vdots & \ddots & 0 & \mathbf{0} \\ 0 & 0 & 0 & \sigma_r^2 & \\ \hdashline \multicolumn{4}{c:}{\mathbf{0}} & \mathbf{0} \end{array}\right]_{n\times n}$$

Gradient-based Learning

- Learning algorithms often seek to minimize/maximize some objective function w.r.t. the model parameter, e.g.

$$\arg\min_{\boldsymbol{w}} J(\boldsymbol{w}) = -E_{\boldsymbol{x},y\sim\hat{p}_{\mathsf{data}}}[\log p_{\mathsf{model}}(y|\boldsymbol{x};\boldsymbol{w})]$$

- Very often, there is no closed-form solution

- Gradient-based learning algorithms are thus called for to update estimates of the solution via an iterative procedure

Steepest Descent

- To decrease $J(\boldsymbol{w})$ in the direction in which it decreases the fastest

$$\boldsymbol{w}^{(n+1)} = \boldsymbol{w}^{(n)} - \epsilon \nabla_{\boldsymbol{w}} J(\boldsymbol{w}^{(n)})$$

  where ϵ controls the step size for each update

- The negative gradient $-\nabla_{\boldsymbol{w}} J(\boldsymbol{w}^{(n)})$ points to the direction in which $J(\boldsymbol{w})$ decreases the fastest at $\boldsymbol{w}^{(n)}$
  - To see this, we define the directional directive at $\boldsymbol{w}_0$ to be

$$\frac{\partial}{\partial \alpha} J(\boldsymbol{w}_0 + \alpha \boldsymbol{u})$$

  - It can then be evaluated as

$$\frac{\partial}{\partial \alpha} J(\boldsymbol{w}_0 + \alpha \boldsymbol{u}) = \boldsymbol{u}^T \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)$$

using the Taylor-1 approximation at $\boldsymbol{w}_0$

$$J(\boldsymbol{w}) \approx J(\boldsymbol{w}_0) + (\boldsymbol{w} - \boldsymbol{w}_0)^T \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)$$

– The unit vector $\boldsymbol{u}$ that points in the direction $-\nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)$ yields a minimal directive among other unit vectors

- Instead of using a fixed ϵ, we can use line search to adapt its value to the curvature of $J(\boldsymbol{w})$ at $\boldsymbol{w}_0$ along $-\nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)$
- This relies on approximating $J(\boldsymbol{w})$ at $\boldsymbol{w}_0$ with Taylor-2 approximation

$$J(\boldsymbol{w}) \approx J(\boldsymbol{w}_0) + (\boldsymbol{w} - \boldsymbol{w}_0)^T \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}_0)^T \boldsymbol{H} (\boldsymbol{w} - \boldsymbol{w}_0)$$

where $\boldsymbol{H}$ is the Hessian matrix defined as

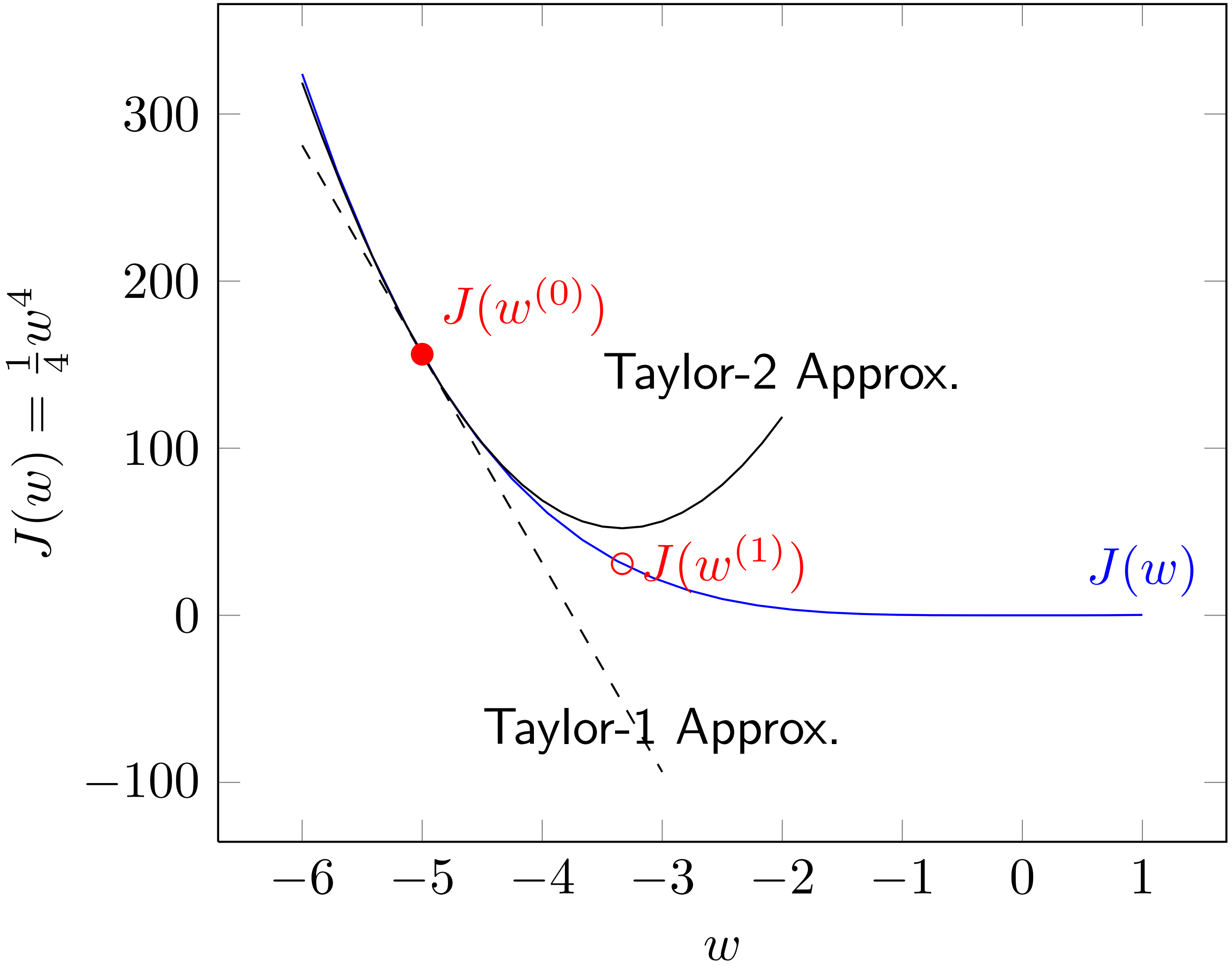
$$\boldsymbol{H}(J(\boldsymbol{w}_0))_{i,j} = \frac{\partial^2}{\partial w_i \partial w_j} J(\boldsymbol{w}_0)$$

- We wish to find an ϵ that maximizes

$$J(\boldsymbol{w}_0) - J(\boldsymbol{w}_0 - \epsilon \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0))$$

- The optimal ϵ is given by

$$\epsilon^* = \frac{\nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)^T \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)}{\nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)^T \boldsymbol{H} \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)}$$


$J(w) = \frac{1}{4}w^4$
300
200
100
0
-100
-6
-5
-4
-3
-2
-1
0
1
w
$J(w^{(0)})$
Taylor-2 Approx.
$J(w^{(1)})$
$J(w)$
Taylor-1 Approx.

Stochastic Gradient Descent (SGD)

- In Steepest Descent, the gradient is computed as

$$\begin{aligned}\boldsymbol{g} &= \nabla_{\boldsymbol{w}} J(\boldsymbol{w}) \\ &= \nabla_{\boldsymbol{w}} \left\{-E_{\boldsymbol{x},y\sim\hat{p}_{\mathsf{data}}}[\log p_{\mathsf{model}}(y|\boldsymbol{x};\boldsymbol{w})]\right\} \\ &= \nabla_{\boldsymbol{w}} \left\{-\frac{1}{m}\sum_{i=1}^{m}\log p_{\mathsf{model}}(y^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{w})\right\} \\ &= -\frac{1}{m}\sum_{i=1}^{m}\nabla_{\boldsymbol{w}}\log p_{\mathsf{model}}(y^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{w})\end{aligned}$$

- SGD uses a minibatch of training examples to approximate the gradient

$$\boldsymbol{g}' = -\frac{1}{m'}\sum_{i=1}^{m'}\nabla_{\boldsymbol{w}}\log p_{\mathsf{model}}(y^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{w})$$

where $m' \ll m$

- Variants of SGD
  - Momentum (Polyak, 1964; DL 8.3.2)
  - Nesterov Momentum (Sutskever et al., 2013; DL 8.3.3)
  - AdaGrad (Duchi et al., 2011; DL 8.5.1)
  - RMSProp (Hinton, 2012; DL 8.5.2)
  - Adam (Kingma and Ba, 2014; DL 8.5.3)

Newton's Method

- To solve for the critical point that minimizes $J(\boldsymbol{w})$ approximated by the Taylor-2 expansion at $\boldsymbol{w_0}$ as the new estimate

$$\arg\min_{\boldsymbol{w}} J(\boldsymbol{w}_0) + (\boldsymbol{w} - \boldsymbol{w}_0)^T \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}_0)^T \boldsymbol{H}(\boldsymbol{w} - \boldsymbol{w}_0)$$

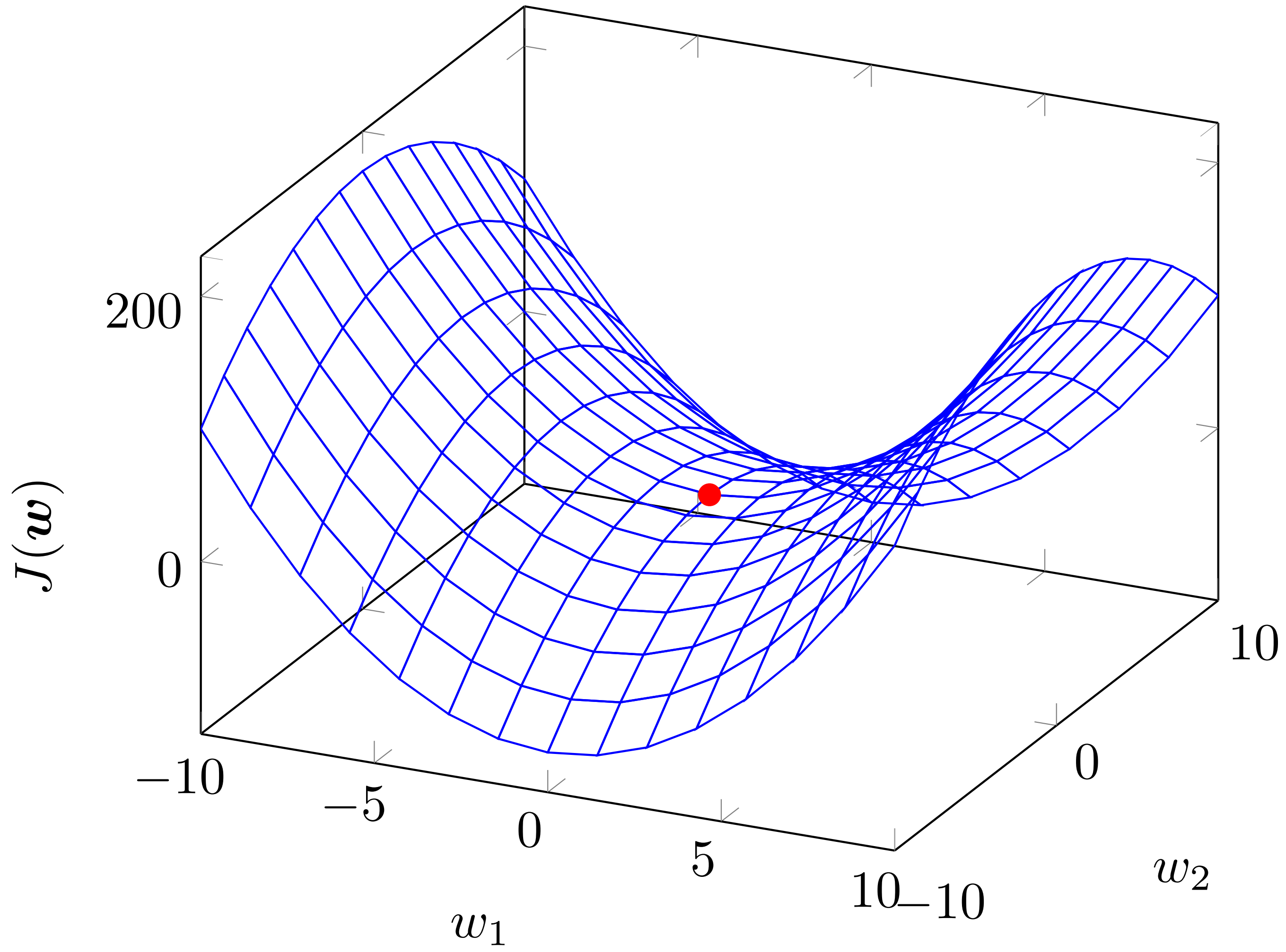
- By setting the gradient w.r.t. $\boldsymbol{w}$ to zero, we have

$$\boldsymbol{w}^* = \boldsymbol{w}_0 - \boldsymbol{H}(J(\boldsymbol{w}_0))^{-1} \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_0)$$

- The iterative update of $\boldsymbol{w}$ then becomes

$$\boldsymbol{w}^{(n+1)} = \boldsymbol{w}^{(n)} - \boldsymbol{H}(J(\boldsymbol{w}^{(n)}))^{-1} \nabla_{\boldsymbol{w}} J(\boldsymbol{w}^{(n)})$$

- The difficulties with training deep learning models using Newton's Method are (1) the need to compute the inverse of the Hessian matrix, and (2) its tendency to be attracted to saddle points



$J(\boldsymbol{w})$
200
0
-10
-5
0
5
10
w_1
-10
0
10
w_2

Example

- We wish to find $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} J(\boldsymbol{w})$, with

$$J(\boldsymbol{w}) = \frac{1}{4}(\boldsymbol{w}^T \boldsymbol{M} \boldsymbol{w})^2, \;\; \boldsymbol{M} = \begin{bmatrix} 6 & -4 \\ -4 & 6 \end{bmatrix}$$

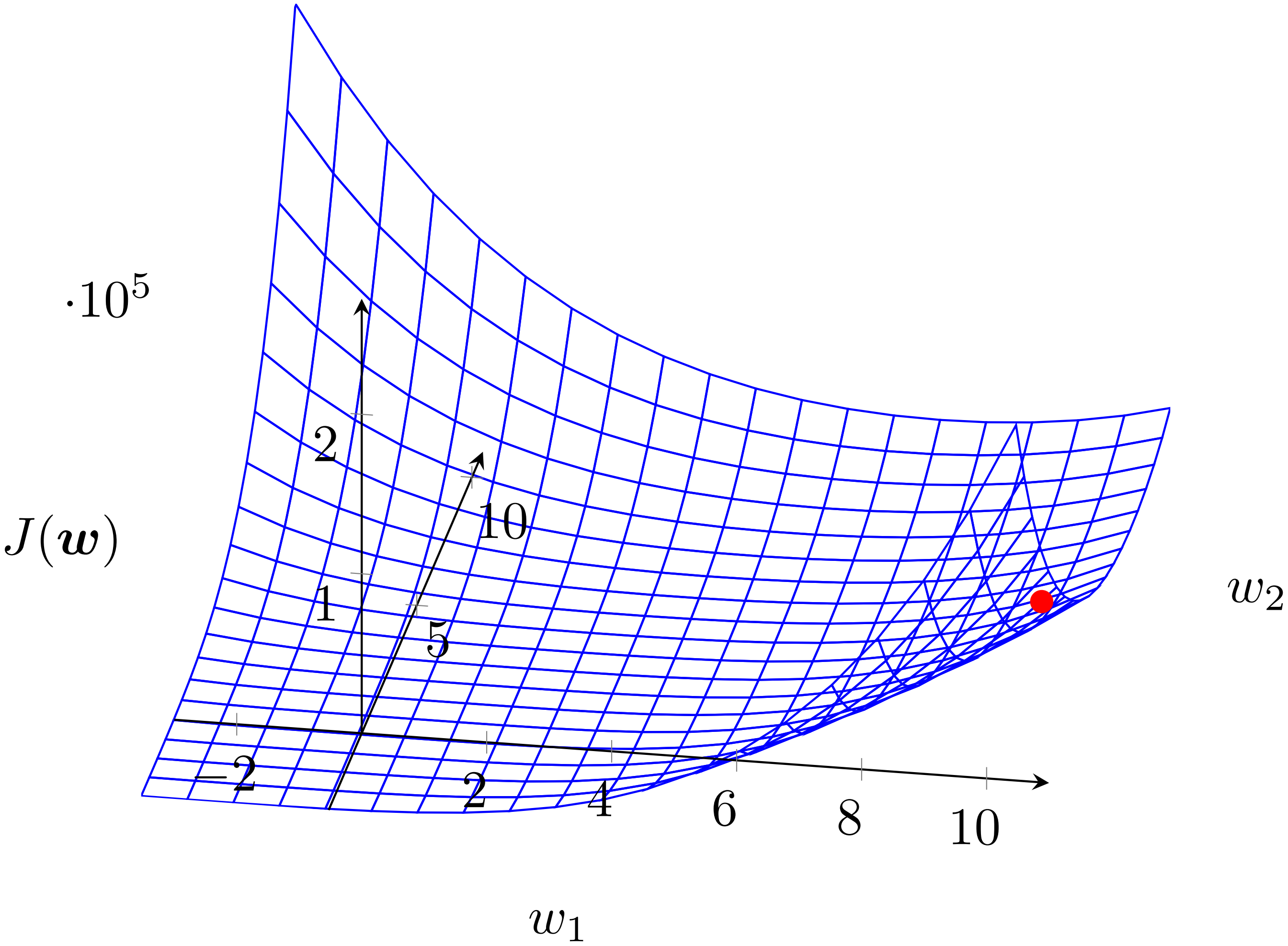
- $\boldsymbol{M}$ has the following pairs of eigenvalues and eigenvectors

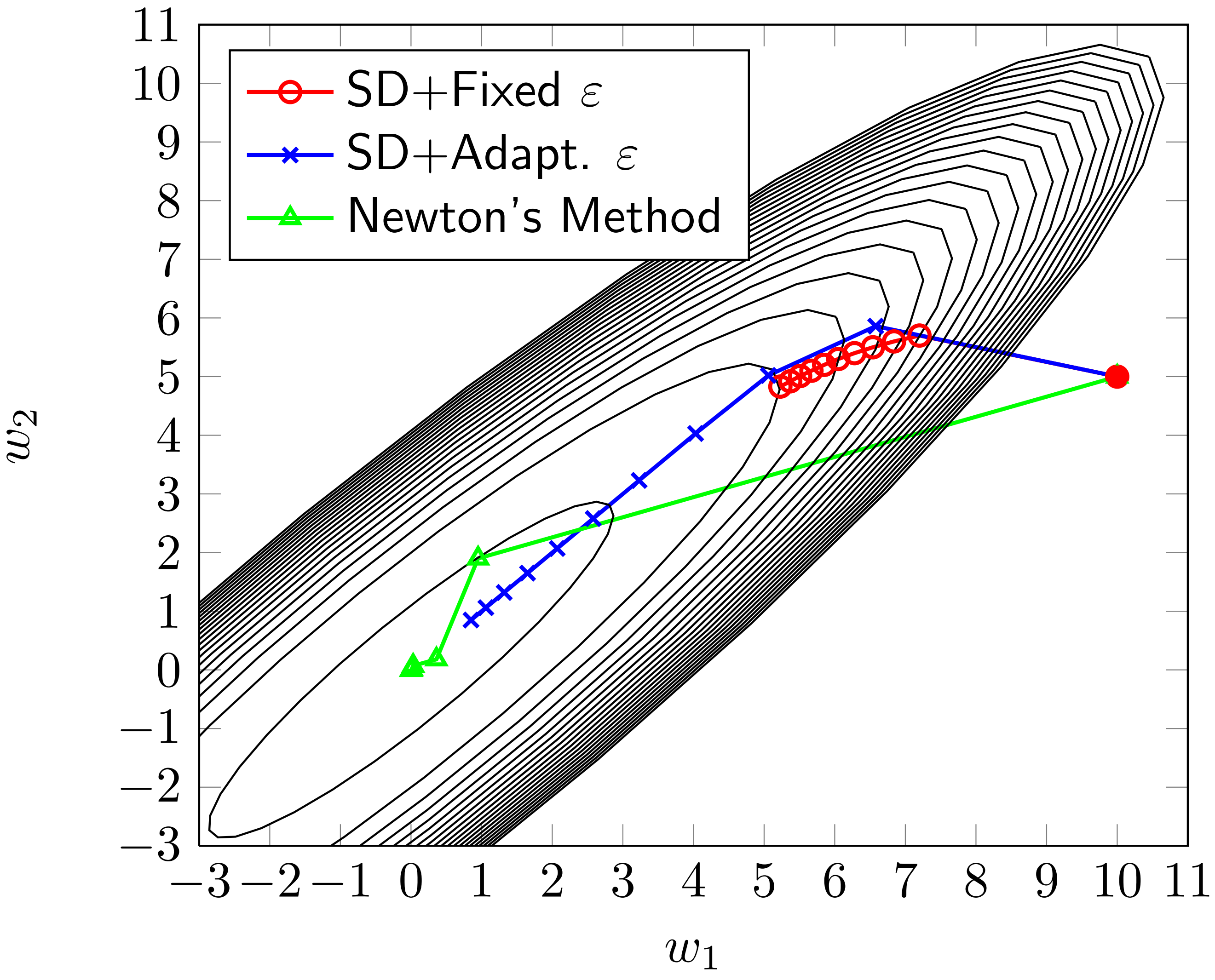
$$\lambda_1 = 1 \rightarrow \boldsymbol{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \;\; \lambda_2 = 5 \rightarrow \boldsymbol{v}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

- The gradient and the Hessian matrix are given by

$$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}) = (\boldsymbol{w}^T \boldsymbol{M} \boldsymbol{w}) \boldsymbol{M} \boldsymbol{w}$$

$$\boldsymbol{H}\{J(\boldsymbol{w})\} = 2\boldsymbol{M}\boldsymbol{w}(\boldsymbol{M}\boldsymbol{w})^T + \boldsymbol{w}^T \boldsymbol{M} \boldsymbol{w} \boldsymbol{M}$$


$\cdot 10^5$
2
1
$J(\boldsymbol{w})$
10
5
-2
2
4
6
8
10
w_1
w_2


SD+Fixed ε
SD+Adapt. ε
Newton's Method
w_1
w_2
−3 −2 −1 0 1 2 3 4 5 6 7 8 9 10 11
11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3

Review

- Overfitting vs. Underfitting
- Generalization
- Regularization
- Estimators (ML vs. MAP)
- Support Vector Machines (SVM)
- Constrained Optimization
- Principle Component Analysis (PCA)
- Gradient-based Learning