CS 559 Machine Learning

Logistic Regression and PCA

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Plan for today

Probabilistic Generative Models

Logistic Regression

Principal Component Analysis

Review of last lecture

- Generative methods vs Discriminative methods
- Linear classifiers: Linear discriminant functions, least square classification, Fisher's linear discriminant (Geometrical properties of Linear Discriminant Analysis), the Perceptron algorithm
- Naive Bayes classifier

Review of gradient descent algorithms

- Three important elements: data($\mathbf{x}, y$), loss function, model parameters $\mathbf{w}$
- One important line, gradient update:

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \nabla \mathbf{w}$$

Gradient Descent

procedure BATCH GRADIENT DESCENT
    for i in range(epochs) **do**
        $g^{(i)}(\mathbf{w}) = \text{evaluate\_gradient}(\text{TrainLoss, data, } \mathbf{w})$
        $\mathbf{w} = \mathbf{w} - \text{learning\_rate} * g^{(i)}(\mathbf{w})$
    end for
end procedure

- Can be very slow.
- Intractable for datasets that don't fit in memory.
- Doesn't allow us to update our model online, i.e. with new examples on-the-fly.
- Guaranteed to converge to the global minimum for convex error surfaces and to a local minimum for non-convex surfaces.

Stochastic Gradient Descent

```
procedure STOCHASTIC GRADIENT DESCENT
    for i in range(epochs) do
        np.random.shuffle(data)
        for example ∈ data do
            g^(i)(w) = evaluate_gradient(loss, example, w)
            w = w − learning_rate * g^(i)(w)
        end for
    end for
end procedure
```

- Allow for online update with new examples.
- With a high variance that cause the objective function to fluctuate heavily.

Mini-batch Gradient Descent

```
procedure MINI-BATCH GRADIENT DESCENT
    for i in range(epochs) do
        np.random.shuffle(data)
        for batch ∈ get_batches(data, batch_size=50) do
            g^(i)(w) = evaluate_gradient(loss, batch, w)
            w = w − learning_rate ∗ g^(i)(w)
        end for
    end for
end procedure
```

- Reduces the variance of the parameter updates, which can lead to more stable convergence;
- Can make use of highly optimized matrix optimizations common to state-of-the-art deep learning libraries that make computing the gradient w.r.t. a mini-batch very efficient.

Evaluation Metrics for Classification

- The contingency table or confusion matrix:

		True value	
		Positive	Negative
Predicted	Positive	True positive (TP)	False positive (FP)
	Negative	False negative (FN)	True negative (TN)

- Recall $= \frac{tp}{tp+fn}$
- Precision $= \frac{tp}{tp+fp}$
- Accuracy $= \frac{tp+tn}{tp+tn+fp+fn}$

Features for Text Classification

- Bag of words: word countings, TFIDF, ...
- Embeddings: word2vec, doc2vec,...
- Domain specific keywords
- Latent variables: topic distributions
- ......

Part I: Probabilistic Generative Models

Probabilistic Generative Models

- We now turn to a probabilistic approach to classification.
- How models with linear decision boundaries arise from simple assumptions about the distribution of the data.

Generative Approach

- Solve the inference problem of estimating the class-conditional densities $p(\mathbf{x}|C_k)$ for each class C_k.
- Infer the prior class probabilities $p(C_k)$.
- Use Bayes' theorem to find the class posterior probabilities:

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})} \tag{1}$$

where

$$p(x) = \sum_k p(\mathbf{x}|C_k)p(C_k) \tag{2}$$

- Use decision theory to determine class membership for each new input $\mathbf{x}$.

Probabilistic Generative Approach-Two Class

Two-class case:

$$
\begin{aligned}
p(C_1|\mathbf{x}) &= \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_1)p(C_1) + p(\mathbf{x}|C_2)p(C_2)} \\
&= \frac{1}{1+e^{-a}} = \sigma(a)
\end{aligned}
\tag{3}
$$

where

$$
a = \ln \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} \tag{4}
$$

$$
\sigma(a) = \frac{1}{1+e^{-a}} \quad \text{(logistic sigmoid function)} \tag{5}
$$

Probabilistic Generative Approach-$K > 2$ Class

$K > 2$ classes:

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{\sum_{j=1}^{K} p(\mathbf{x}|C_j)p(C_j)} = \frac{e^{a_k}}{\sum_{j=1}^{K} e^{a_j}} \tag{6}$$

where

$$a_k = \ln\ p(\mathbf{x}|C_k)p(C_k) \tag{7}$$

$$\sigma(a) = \frac{e^{a_k}}{\sum_{j=1}^{K} e^{a_j}} \quad \text{(softmax function)} \tag{8}$$

Probabilistic Generative Models

- Lets assume the class-conditional densities are Gaussian with the same covariance matrix:

$$p(\mathbf{x}|C_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} e^{\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu}_k)\right)} \tag{9}$$

- Two class case first. We can show the following result:

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x} + \omega_0) \tag{10}$$

$$\mathbf{w} = \Sigma^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \tag{11}$$

$$\omega_0 = -\frac{1}{2}\boldsymbol{\mu}_1^T \Sigma \boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T \Sigma \boldsymbol{\mu}_2 + \ln \frac{p(C_1)}{p(C_2)} \tag{12}$$

- How?

Probabilistic Generative Models

$$P(C_1|\mathbf{x}) = \sigma(a) = \frac{1}{1+e^{-a}} \tag{13}$$

$$\begin{aligned} a &= \ln p(\mathbf{x}|C_1) - \ln p(\mathbf{x}|C_2) + \ln \frac{p(C_1)}{p(C_2)} \rightarrow \text{(Replace } p(\mathbf{x}|C_k)) \\ &= -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_1) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_2)^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_2) \\ &+ \ln \frac{p(C_1)}{p(C_2)} \end{aligned} \tag{14}$$

Probabilistic Generative Models

$$
\begin{aligned}
a &= -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_1) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_2)^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_2) + \ln\frac{p(C_1)}{p(C_2)} \\
&= -\frac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x} + \frac{1}{2}\boldsymbol{\mu}_1^T\Sigma^{-1}\mathbf{x} + \frac{1}{2}\mathbf{x}^T\Sigma^{-1}\boldsymbol{\mu}_1 - \frac{1}{2}\boldsymbol{\mu}_1^T\Sigma^{-1}\boldsymbol{\mu}_1 \\
&+ \frac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}_2^T\Sigma^{-1}\mathbf{x} - \frac{1}{2}\mathbf{x}^T\Sigma^{-1}\boldsymbol{\mu}_2 + \frac{1}{2}\boldsymbol{\mu}_2^T\Sigma^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(C_1)}{p(C_2)} \\
&= \boldsymbol{\mu}_1^T\Sigma^{-1}\mathbf{x} - \boldsymbol{\mu}_2^T\Sigma^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}_1^T\Sigma^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T\Sigma^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(C_1)}{p(C_2)} \\
&= (\boldsymbol{\mu}_1-\boldsymbol{\mu}_2)^T\Sigma^{-1}\mathbf{x} + \omega_0 = \mathbf{w}^T\mathbf{x} + \omega_0 \qquad (15)
\end{aligned}
$$

Thus:

$$
\mathbf{w} = \Sigma^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \qquad (16)
$$

Probabilistic Generative Models

- We have shown:

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + \omega_0)$$
$$\mathbf{w} = \Sigma^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$
$$\omega_0 = -\frac{1}{2}\boldsymbol{\mu}_1^T\Sigma\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T\Sigma\boldsymbol{\mu}_2 + \ln\frac{p(C_1)}{p(C_2)}$$

- Decision boundary:

$$p(C_1|\mathbf{x}) = p(C_2|\mathbf{x}) = 0.5 \tag{17}$$

$$\Rightarrow \frac{1}{1 + e^{-(\mathbf{w}^T\mathbf{x}+\omega_0)}} = 0.5 \Rightarrow \mathbf{w}^T\mathbf{x} + \omega_0 = 0 \tag{18}$$

Probabilistic Generative Models

- $\underline{K > 2 \text{ classes}}$:

$$P(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{\sum_j p(\mathbf{x}|C_j)p(C_j)} = \frac{e^{a_k}}{\sum_j e^{a_j}} \tag{19}$$

$$a_k = \ln\ p(\mathbf{x}|C_k)p(C_k) \tag{20}$$

- We can show the following result:

$$p(C_k|\mathbf{x}) = \frac{e^{\mathbf{w}_k^T\mathbf{x}+\omega_{k0}}}{\sum_j e^{\mathbf{w}_j^T\mathbf{x}+\omega_{j0}}} \tag{21}$$

$$\mathbf{w}_k = \Sigma^{-1}\boldsymbol{\mu}_k \tag{22}$$

$$\omega_{k0} = -\frac{1}{2}\boldsymbol{\mu}_k^T\Sigma^{-1}\boldsymbol{\mu}_k + \ln\ p(C_k) \tag{23}$$

Maximum Likelihood Solution

- We have a parametric functional form for the class-conditional densities:

$$p(\mathbf{x}|C_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} e^{\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu}_k)\right)} \tag{24}$$

- We can estimate the parameters and the prior class probabilities using maximum likelihood.
  - Two class case with shared covariance matrix.
  - Training data:

$$\{\mathbf{x}_n, y_n\}, \quad n = 1, ..., N$$

$y_n = 1$ denotes class C_1; $y_n = 0$ denotes class C_2;

Priors: $p(C_1) = \gamma, p(C_2) = 1 - \gamma$

Maximum Likelihood Solution

- For a data point $\mathbf{x}_n$ from class C_1, we have $y_n = 1$ and therefore:

$$p(\mathbf{x}_n, C_1) = p(\mathbf{x}|C_1)p(C_1) = \gamma\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma) \tag{25}$$

- For a data point $\mathbf{x}_n$ from class C_1, we have $y_n = 1$ and therefore:

$$p(\mathbf{x}_n, C_2) = p(\mathbf{x}|C_2)p(C_2) = (1-\gamma)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma) \tag{26}$$

- Assuming observations are drawn independently, the likelihood function is as below:

$$\begin{aligned} p(\mathcal{D}|\gamma, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma) &= \prod_{n=1}^{N} \left[p(\mathbf{x}_n, C_1)\right]^{y_n} \left[p(\mathbf{x}_n, C_2)\right]^{1-y_n} \\ &= \prod_{n=1}^{N} \left[\gamma\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right]^{y_n} \left[(1-\gamma)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right]^{1-y_n} \end{aligned}$$

Maximum Likelihood Solution

- We want to find the values of the parameters that **maximize the likelihood function**, i.e., fit a model that best describes the observed data.

$$p(\mathcal{D}|\gamma, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma) = \prod_{n=1}^{N} \left[\gamma \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right]^{y_n} \left[(1-\gamma)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right]^{1-y_n} \tag{27}$$

- As usual, we consider the log of the likelihood:

$$\begin{aligned} &\ln\, p(\mathcal{D}|\gamma, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma) = \\ &\sum_{n=1}^{N} \left[y_n \ln\gamma + y_n \ln\, \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right. \\ &\left. + (1-y_n)\ln\, (1-\gamma) + (1-y_n)\ln\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right] \end{aligned} \tag{28}$$

Maximum Likelihood Solution - parameter γ

$$\ln p(\mathcal{D}|\gamma,\boldsymbol{\mu}_1,\boldsymbol{\mu}_2,\Sigma) = \sum_{n=1}^{N} \big[y_n \ln \gamma + y_n \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1,\Sigma) + (1-y_n)\ln(1-\gamma) + (1-y_n)\ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2,\Sigma) \big]$$

- We first maximize the log-likelihood with respect to γ (set derivate to 0)

$$\gamma = \frac{1}{N}\sum_{n=1}^{N} y_n = \frac{N_1}{N} = \frac{N_1}{N_1+N_2} \tag{29}$$

- The maximum likelihood estimate of γ is the fraction of points in class C_1.
- For multi-class: ML estimate for $p(C_k)$ is given by the fraction of points in the training set in C_k.

Maximum Likelihood Solution - parameter $\boldsymbol{\mu}$

$$\ln p(\mathcal{D}|\gamma,\boldsymbol{\mu}_1,\boldsymbol{\mu}_2,\Sigma) = \sum_{n=1}^{N}\Big[y_n \ln\gamma + y_n \ln\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1,\Sigma) + (1-y_n)\ln(1-\gamma) + (1-y_n)\ln\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2,\Sigma)\Big]$$

- We them maximize the log-likelihood with respect to $\boldsymbol{\mu}_1$ (set derivate to 0)

$$\boldsymbol{\mu}_1 = \frac{1}{N_1}\sum_{n=1}^{N} y_n\mathbf{x}_n \qquad (30)$$

- The maximum likelihood estimate of $\boldsymbol{\mu}_1$ is the sample mean of all input $\mathbf{x}_n$ in class C_1.
- The maximum likelihood estimate of μ_2 is:

$$\boldsymbol{\mu}_2 = \frac{1}{N_2}\sum_{n=1}^{N}(1-y_n)\mathbf{x}_n \qquad (31)$$

Maximum Likelihood Solution - parameter Σ

- Maximize the log-likelihood with respect to Σ (set derivate to 0), we obtain the estimate Σ_{ML}

$$\Sigma_{ML} = \frac{N_1}{N} S_1 + \frac{N_2}{N} S_2 \tag{32}$$

where

$$S_1 = \frac{1}{N_1} \sum_{n \in C_1} (\mathbf{x}_n - \boldsymbol{\mu}_1)(\mathbf{x}_n - \boldsymbol{\mu}_1)^T \tag{33}$$

$$S_2 = \frac{1}{N_2} \sum_{n \in C_2} (\mathbf{x}_n - \boldsymbol{\mu}_2)(\mathbf{x}_n - \boldsymbol{\mu}_2)^T \tag{34}$$

- The maximum likelihood estimate of the covariance is given by the weighted average of the sample covariance matrices associated with each of the classes.
- The results extend to K classes.

Summary so far

- We assumed $p(\mathbf{x}|(y=1)) \sim \mathcal{N}(\boldsymbol{\mu}_+, \Sigma_+)$ and $p(\mathbf{x}|(y=-1)) \sim \mathcal{N}(\boldsymbol{\mu}_-, \Sigma_-)$, and two class-probabilities $p(y=1)$ and $p(y=-1)$.

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- This is called an generative model, as we have written down a full joint model over the data.

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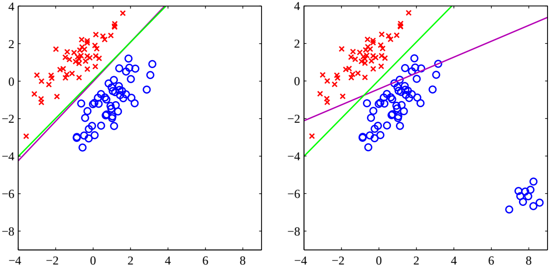
- This is called an generative model, as we have written down a full joint model over the data.
- We saw that violations of the model assumption can lead to "bad" decision boundaries.



Figures from Bishop PRML, 44a and b

Probabilistic Generative Models - parameters

- How many parameters did we estimate to fit Gaussian class-conditional densities (the generative approach)?

$$
\begin{aligned}
p(C_1) &\Rightarrow 1 \\
\text{2 mean vectors } &\Rightarrow 2d \\
\Sigma &\Rightarrow d + \frac{d^2 - d}{2} = \frac{d^2 + d}{2} \\
\text{total } &= 1 + 2d + \frac{d^2 + d}{2} = O(d^2)
\end{aligned}
$$

Part II: Logistic Regression

Logistic Regression

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + \omega_0) = f(\mathbf{x}) \tag{35}$$

- We use maximum likelihood to determine the parameters of the logistic regression model.

$$\{\mathbf{x}_n, y_n\}, \quad n = 1, ..., N$$

$$y_n = 1 \text{ denotes class } C_1; \; y_n = 0 \text{ denotes class } C_2;$$

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- We want to find the values of **w** that maximize the posterior probabilities associated to the observed data
- Likelihood function:

$$\begin{aligned} L(\mathbf{w}) &= \prod_{n=1}^{N} p(C_1|\mathbf{x}_n)^{y_n}(1 - p(C_1|\mathbf{x}_n))^{1-y_n} \\ &= \prod_{n=1}^{N} f(\mathbf{x}_n)^{y_n}(1 - f(\mathbf{x}_n))^{1-y_n} \end{aligned} \tag{36}$$

Logistic Regression

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + \omega_0) = f(\mathbf{x})$$

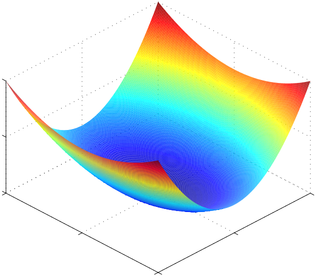
- We consider the negative logarithm of the likelihood (Cross Entropy):

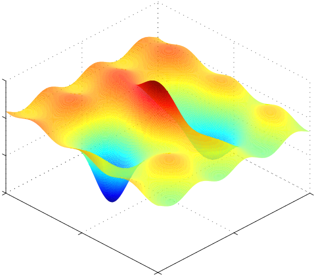
$$\begin{aligned} E(\mathbf{w}) = -\ln\ L(\mathbf{w}) &= -\ln\ \prod_{n=1}^{N} p(C_1|\mathbf{x}_n)^{y_n}(1 - p(C_1|\mathbf{x}_n))^{1-y_n} \\ &= -\sum_{n=1}^{N}(y_n \ln f(\mathbf{x}_n) + (1 - y_n)\ln\ (1 - f(\mathbf{x}_n))) \end{aligned} \tag{37}$$

- Thus:

$$\max L(\mathbf{w}) = \min E(\mathbf{w}) \tag{38}$$

The cost-function for logistic regression is convex.





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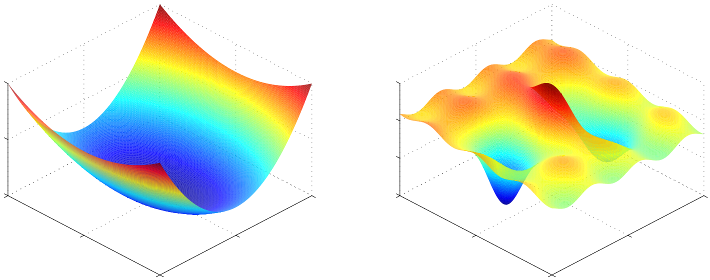

- Fact: The negative log-likelihood is *convex* – this makes life much more easier.

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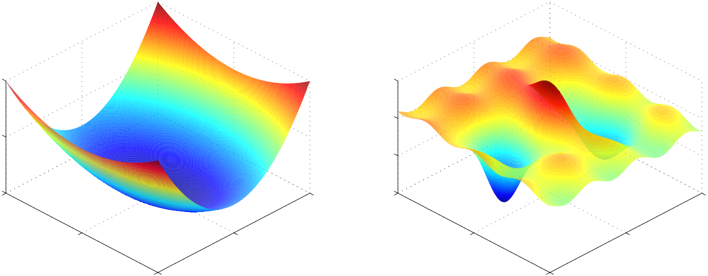

- Fact: The negative log-likelihood is *convex* – this makes life much more easier.
- There are no local minima to get stuck in, and there is good optimization techniques for convex problems.

Logistic Regression - Gradient

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + \omega_0) = f(\mathbf{x})$$

- We compute the derivative of the error function with respect to **w**

$$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \frac{\partial}{\partial \mathbf{w}}\left[-\ln \prod_{n=1}^{N} p(C_1|\mathbf{x}_n)^{y_n}(1 - p(C_1|\mathbf{x}_n))^{1-y_n}\right] \quad (39)$$

- The derivative of the logistic sigmoid function:

$$\begin{aligned} \frac{\partial}{\partial a}\sigma(a) &= \frac{\partial}{\partial a}\frac{1}{1+e^{-a}} = \frac{e^{-a}}{(1+e^{-a})^2} \\ &= \frac{1}{1+e^{-a}}\frac{e^{-a}}{(1+e^{-a})} = \frac{1}{1+e^{-a}}(1 - \frac{1}{1+e^{-a}}) \\ &= \sigma(a)(1-\sigma(a)) \end{aligned} \quad (40)$$

Logistic Regression

Homework: The derivative of the error function with respect to $\mathbf{w}$ is:

$$\nabla_{\mathbf{w}} E(\mathbf{w}) = \sum_{n=1}^{N} (f(\mathbf{x}) - y_n)\mathbf{x}_n \tag{41}$$

Probabilistic Discriminative Models - parameters

- Two-class case:

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + \omega_0) = f(\mathbf{x})$$

$$P(C_2|\mathbf{x}) = 1 - P(C_1|\mathbf{x})$$

- This model is know as Logistic Regression.
- Assuming $\mathbf{x} \in \mathbb{R}^d$, how many parameters do we need to estimate?

$$d + 1$$

Summary so far

- From the previous introduction, we know that

$$P(y = 1|\mathbf{x}) = \sigma(a(\mathbf{x}))$$

where $\sigma(a) = 1/(1 + \exp(-a))$ and $a(x) = \mathbf{w}^\top \mathbf{x} + \omega_o$.
- Notation is simpler if we use 0 and 1 as class labels, so we define $y_n = 1$ as the label for the positive class, and $y_n = 0$ as label for the negative class.
- In other words, $y|x \sim \text{Bernoulli}(\sigma(f(x)))$.

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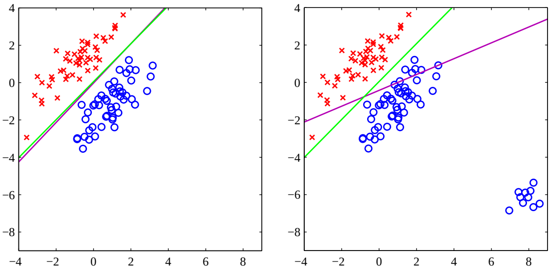
- This is a discriminative approach to classification, as we only model the labels, and not the inputs.
- Decision rule and function shape of $p(y|\mathbf{x})$ will be the same for the generative and the discriminative model, but the parameters were obtained differently.

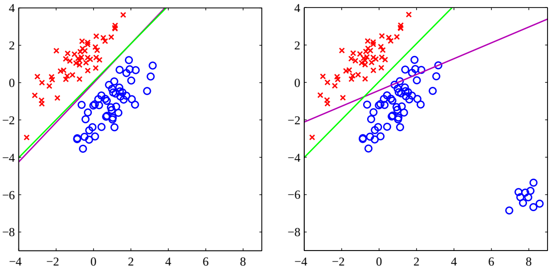
Maximum likelihood estimation of Logistic Regression



Bishop PRML Figure 44 a and b

- Logistic regression is a *much* better algorithm than the algorithms we discussed last week.
- Need to optimize log-likelihood numerically.

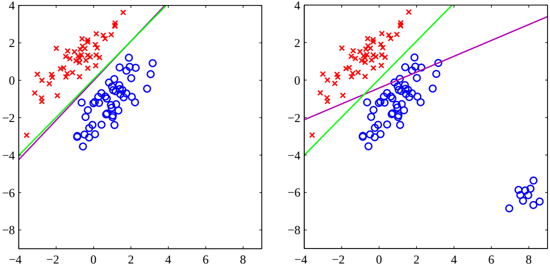
Maximum likelihood estimation of Logistic Regression



Bishop PRML Figure 44 a and b

- Logistic regression is a *much* better algorithm than the algorithms we discussed last week.
- Need to optimize log-likelihood numerically.
- People typically minimize the negative log-likelihood $\mathcal{L}$ rather than maximize the log-likelihood...

Maximum likelihood estimation of Logistic Regression



Bishop PRML Figure 44 a and b

- Logistic regression is a *much* better algorithm than the algorithms we discussed last week.
- Need to optimize log-likelihood numerically.
- People typically minimize the negative log-likelihood $\mathcal{L}$ rather than maximize the log-likelihood...
- To numerically minimize the negative log-likelihood, we need its gradient (and maybe its hessian)

Multiclass Logistic Regression

- Multiclass case:

$$p(C_k|\mathbf{x}) = \frac{e^{\mathbf{w}_k^T\mathbf{x}+\omega_{k0}}}{\sum_j e^{\mathbf{w}_j^T\mathbf{x}+\omega_{j0}}} = f_k(\mathbf{x}) \quad (42)$$

- We use maximum likelihood to determine the parameters:

$$\{\mathbf{x}_n, y_n\}, \quad n = 1, ..., N$$

$$y_n = (0, ..., 1, ..., 0) \text{ denotes class } C_k$$

- We want to find the values of $\mathbf{w}_1, ..., \mathbf{w}_k$ that maximize the posterior probabilities associated to the observed data likelihood function:

$$\mathcal{L}(\mathbf{w}_1, ..., \mathbf{w}_k) = \prod_{n=1}^{N}\prod_{k=1}^{K} p(C_k|\mathbf{x}_n)^{y_{nk}} = \prod_{n=1}^{N}\prod_{k=1}^{K} f_k(\mathbf{x}_n)^{y_{nk}} \quad (43)$$

Multiclass Logistic Regression

$$\mathcal{L} = \prod_{n=1}^{N} \prod_{k=1}^{K} p(C_k|\mathbf{x}_n)^{y_{nk}} = \prod_{n=1}^{N} \prod_{k=1}^{K} f_k(\mathbf{x}_n)^{y_{nk}}$$

- Consider the negative logarithm of the likelihood:

$$\mathcal{E}(\mathbf{w}_1, ..., \mathbf{w}_k) = -\ln\mathcal{L}(\mathbf{w}_1, ..., \mathbf{w}_k) = -\sum_{n=1}^{N} \sum_{k=1}^{K} y_{nk} \ln f_k(\mathbf{x}_n) \quad (44)$$

$$\min_{\mathbf{w}_j} \mathcal{E}((\mathbf{w}_j)) \quad (45)$$

- The gradient of the error function w.r.t one of the parameter vectors:

$$\frac{\partial}{\partial \mathbf{w}_j}\mathcal{E}(\mathbf{w}_1, ..., \mathbf{w}_k) = \frac{\partial}{\partial \mathbf{w}_j}\Big[-\sum_{n=1}^{N} \sum_{k=1}^{K} y_{nk} \ln\ f_k(\mathbf{x}_n)\Big] \quad (46)$$

Multiclass Logistic Regression

$$\frac{\partial}{\partial \mathbf{w}_j}\mathcal{E}(\mathbf{w}_1, ..., \mathbf{w}_k) = \frac{\partial}{\partial \mathbf{w}_j}\Big[- \sum_{n=1}^{N}\sum_{k=1}^{K} y_{nk} \ln\ f_k(\mathbf{x}_n)\Big]$$

- The derivatives of the softmax function:

$$\frac{\partial}{\partial a_k} f_k = \frac{\partial}{\partial a_k} \frac{e^{a_k}}{\sum_j e^{a_j}} = \frac{e^{a_k}\sum_j e^{a_j} - e^{a_k}e^{a_k}}{(\sum_j e^{a_j})^2} = f_k - f_k^2 = f_k(1 - f_k)$$

- Thus:

$$\text{for } j \neq k, \frac{\partial}{\partial a_j} f_k = \frac{\partial}{\partial a_j} f_k = \frac{\partial}{\partial a_j} \frac{e^{a_k}}{\sum_j e^{a_j}} = \frac{-e^{a_k}e^{a_j}}{(\sum_j e^{a_j})^2} = -f_k f_j$$

- Compact expression (I_{kj} are the elements of the identity matrix)

$$\frac{\partial}{\partial a_j} f_k = f_k(I_{kj} - f_j)$$

Multiclass Logistic Regression

$$\nabla_{\mathbf{w}_j}\mathcal{E}(\mathbf{w}_1, \ldots, \mathbf{w}_k) = \sum_{n=1}^{N}(f_{nj} - y_{nj})\mathbf{x}_n$$

Multiclass Logistic Regression

$$\nabla_{\mathbf{w}_j}\mathcal{E}(\mathbf{w}_1, ..., \mathbf{w}_k) = \sum_{n=1}^{N}(f_{nj} - y_{nj})\mathbf{x}_n$$

- It can be shown that $\mathcal{E}$ is a convex function of $\mathbf{w}$. Thus, it has a unique minimum.
- For a batch solution, we can use the Newton-Raphson optimization technique.
- Online solution (SGD):

$$\mathbf{w}_j^{t+1} = \mathbf{w}_j^t - \eta\nabla_{\mathbf{w}_j}\mathcal{E}_n(\mathbf{w}) = \mathbf{w}_j^t - \eta(f_{nj} - y_{nj})\mathbf{x}_n$$

Part III: PCA

Eigenvalues and Eigenvectors

- For an $n \times n$ square matrix A, $\mathbf{e}$ is an eigenvector with eigenvalue λ if:

$$A\mathbf{e} = \lambda\mathbf{e}$$

or

$$(A - \lambda I)\mathbf{e} = 0$$

- If $(A - \lambda I)$ is invertible, the only solution is $\mathbf{e} = \mathbf{0}$ (trivial).

Eigenvalues and Eigenvectors

- For non-trivial solutions

$$det(A - \lambda I) = 0$$

- This is called the "characteristic polynomial"
- Solutions are not unique because if $\mathbf{e}$ is an eigenvector $a\mathbf{e}$ is also an eigenvector.

Eigenvalues and Eigenvectors - simple example

- For a 2×2 matrix A:
$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$$
- Given:
$$det(A - \lambda I) = \begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = (a_{11} - \lambda)(a_{22} - \lambda) - a_{12}a_{21} = 0$$
- We get: $a_{11}a_{22} - a_{12}a_{21} - (a_{11} + a_{22})\lambda + \lambda^2 = 0 \rightarrow$
$1 \cdot 4 - 2 \cdot 2 - (1 + 4)\lambda + \lambda^2 = 0$
- Solutions are $\lambda = 0$ and $\lambda = 5$.

Eigenvalues and Eigenvectors - simple example

- The eigenvector for the first eigenvalue, $\lambda = 0$ is:

$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1x + 2y \\ 2x + 4y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

- One solution for both equations is $x = 2, y = -1$
- The eigenvector for the second eigenvalue, $\lambda = 5$ is:

$$\begin{bmatrix} -4 & 2 \\ 2 & -1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -4x + 2y \\ 2x - 1y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

- One solution for both equations is $x = 1, y = 2$

Eigenvalues and Eigenvectors - properties

- The product of the eigenvalues is the determinant of A: $det(A)$
- The sum of the eigenvalues $=$ trace(A)
- The eigenvectors are pairwise orthogonal

Dimensionality Reduction

- Many dimensions are often interdependent (correlated);
- Solution 1: reduce the dimensionality of problems;
- Solution 2: transform interdependent coordinates into significant and independent ones;

Principal Component Analysis

It is also called Karhunen-Loeve transformation

- PCA transforms the original input space into a lower dimensional space, by constructing dimensions that are linear combinations of the given features;
- The objective is to consider independent dimensions along which data have largest variance (i.e., greatest variability)

Principal Component Analysis

- PCA involves a linear algebra procedure that transforms a number of possibly correlated variables into a smaller number of uncorrelated variables called principal components;
- The first principal component accounts for as much of the variability in the data as possible;
- Each succeeding component (orthogonal to the previous ones) accounts for as much of the remaining variability as possible.

Principal Component Analysis

- So: PCA finds n linearly transformed components, $s_1, s_2, ..., s_n$, so that they explain the maximum amount of variance;
- We can define PCA in an intuitive way using a recursive formulation:

Principal Component Analysis

- Suppose data are first centered at the origin (i.e., their mean is $\mathbf{0}$)
- We define the direction of the first principal component, say, $\mathbf{w}_1$ as follows:

$$\mathbf{w}_1 = \arg\max_{||\mathbf{w}||=1} E[(\mathbf{w}^T\mathbf{x})^2]$$

  where $\mathbf{w}_1$ is of the same dimensionality d as the data vector $\mathbf{x}$.
- Thus: the first principal component is the projection on the direction along which the variance of the projection is maximized.

Principal Component Analysis

- Having determined the first $k-1$ principal components, the k-th principal component is determined as the principal component of the data residual:

$$\mathbf{w}_k = \arg\max_{||\mathbf{w}||=1} E\{[\mathbf{w}^T(\mathbf{x} - \sum_{i=1}^{k-1} \mathbf{w}_i \mathbf{w}_i^T \mathbf{x})]^2\}$$

- The principal components are then given by:

$$s_i = \mathbf{w}_i^T \mathbf{x}$$

Simple illustration of Principal Component Analysis

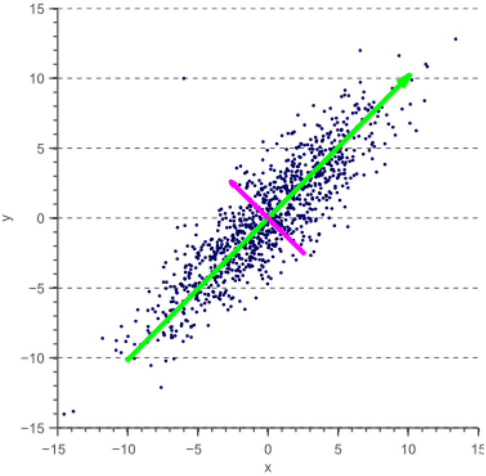


Figure: Green: first principal component of a two-dimensional dataset; Magenta: second principal component

PCA - Geometric interpretation

PCA rotates the data (centered at the origin) in such a way that the maximum variability is visible (i.e., aligned with the axes.)

PCA - How to compute the principal components

- Let $\mathbf{w}$ be the direction of the first principal component, with $||\mathbf{w}|| = 1$
- $s_i = \mathbf{w}^T \mathbf{x}_i$ is the projection of $\mathbf{x}_i$ along $\mathbf{w}$.
- $\bar{s} = \frac{1}{N} \sum_{i=1}^{N} s_i = \frac{1}{N} \sum_{i=1}^{N} \mathbf{w}^T \mathbf{x}_i$
- Variance of data along $\mathbf{w}$:

$$\frac{1}{N} \sum_{i=1}^{N} (s_i - \bar{s})^2 = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{w}^T \mathbf{x}_i - \frac{1}{N} \sum_{j=1}^{N} \mathbf{w}^T \mathbf{x}_j)^2$$

PCA - How to compute the principal components

$$
\begin{aligned}
\frac{1}{N}\sum_{i=1}^{N}(s_i - \bar{s})^2 &= \frac{1}{N}\sum_{i=1}^{N}(\mathbf{w}^T\mathbf{x}_i - \frac{1}{N}\sum_{j=1}^{N}\mathbf{w}^T\mathbf{x}_j)^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left[\mathbf{w}^T\;(\mathbf{x}_i - \frac{1}{N}\sum_{j=1}^{N}\mathbf{x}_j)\right]^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left[\mathbf{w}^T(\mathbf{x}_i - \bar{\mathbf{x}})\right]^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left[\mathbf{w}^T(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T\mathbf{w}\right] \\
&= \mathbf{w}^T\underbrace{\left\{\frac{1}{N}\sum_{i=1}^{N}\left[(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T\right]\right\}}_{\text{sample covariance matrix}}\mathbf{w} \\
&= \mathbf{w}^T\Sigma\mathbf{w}
\end{aligned}
$$

PCA - How to compute the principal components

- Thus, the variance of data along direction $\mathbf{w}$ can be written as:

$$\mathbf{w}^T \Sigma \mathbf{w}$$

- Our objective is to find $\mathbf{w}$ such that:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \mathbf{w}^T \Sigma \mathbf{w}$$

  with the constraint $\mathbf{w}^T \mathbf{w} = 1$

- By introducing one Lagrange multiplier λ we obtain the following unconstrained optimization problem:

$$\mathbf{w} = \arg\max_{\mathbf{w}} [\mathbf{w}^T \Sigma \mathbf{w} - \lambda(\mathbf{w}^T \mathbf{w} - 1)]$$

- Setting $\frac{\partial}{\partial \mathbf{w}} = 0$, gives $2\Sigma\mathbf{w} - 2\lambda\mathbf{w} = 0$
- That is $\Sigma\mathbf{w} = \lambda\mathbf{w}$ (reduced to an eigenvalue problem)

PCA - How to compute the principal components

The solution $\mathbf{w}$ is the eigenvector of Σ corresponding to the largest eigenvalue λ:

$$\Sigma \mathbf{w} = \lambda \mathbf{w}$$

PCA - Summary

- The computation of the $\mathbf{w}_i$ is accomplished by solving an eigenvalue problem for the sample covariance matrix (assuming data have 0 mean):

$$\Sigma = E[\mathbf{x}\mathbf{x}^T]$$

- The eigenvector associated with the largest eigenvalue corresponds to the first principal component; the eigenvector associated with the second largest eigenvalue corresponds to the second principal component; and so on...
- Thus: The $\mathbf{w}_i$ are the eigenvectors of Σ that correspond to the i largest eigenvalues of Σ.

PCA - In practice

- The basic goal of PCA is to reduce the dimensionality of the data. Thus, one usually chooses:

$$n \ll d$$

- But how do we select the number of components n?

Determining the number of component

- Plot the eigenvalues–each eigenvalue is related to the amount of variation explained by the corresponding axis (eigenvector);
- If the points on the graph tend to level out (show an "elbow" shape), these eigenvalues are usually close enough to zero that they can be ignored;
- In general: Limit the variance accounted for.

Determining the number of component

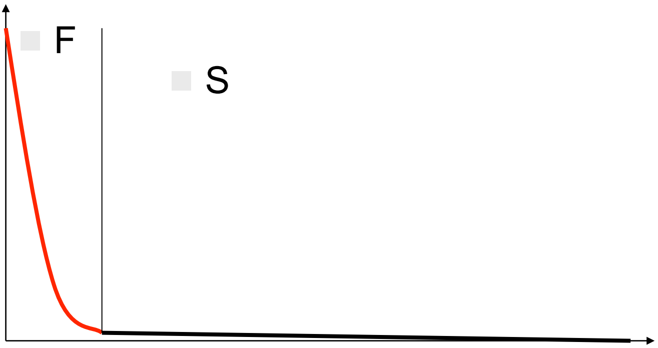
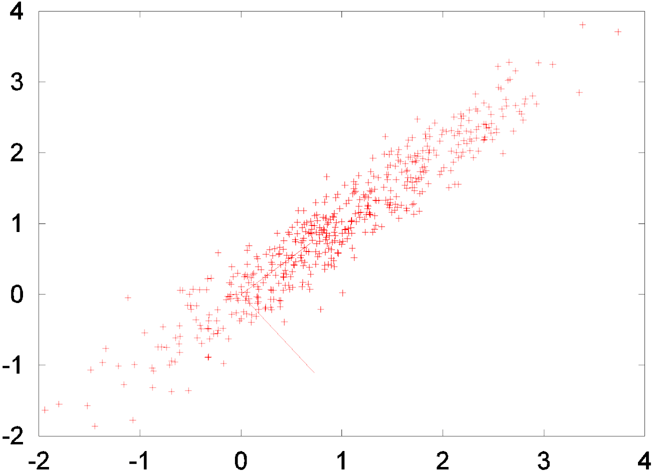


Figure: A typical eigenvalue spectrum and its division into two orthogonal subspaces

Determining the number of component



$$\lambda_1 = 1.98, \quad \lambda_2 = 0.05$$

Determining the number of component

- $\mathbf{x}_i \in \mathbb{R}^d, i = 1, ..., N$
- $\mathbf{w}_1, \mathbf{w}_2, ..., \mathbf{w}_d$: d eigenvectors (principal component directions)
- $||\mathbf{w}_i|| = 1$ (the $\mathbf{w}_i$s are orthonormal vectors)
- Representation of $\mathbf{x}_i$ in eigenvector space:

$$\mathbf{z}_i = (\mathbf{w}_1^T \mathbf{x}_i)\mathbf{w}_1 + (\mathbf{w}_2^T \mathbf{x}_i)\mathbf{w}_2 + ... + (\mathbf{w}_d^T \mathbf{x}_i)\mathbf{w}_d$$

- Suppose we retain the first k principal component:

$$\mathbf{z}_i^k = (\mathbf{w}_1^T \mathbf{x}_i)\mathbf{w}_1 + (\mathbf{w}_2^T \mathbf{x}_i)\mathbf{w}_2 + ... + (\mathbf{w}_k^T \mathbf{x}_i)\mathbf{w}_k$$

- Then:

$$\mathbf{z}_i - \mathbf{z}_i^k = (\mathbf{w}_{k+1}^T \mathbf{x}_i)\mathbf{w}_{k+1} + ... + (\mathbf{w}_d^T \mathbf{x}_i)\mathbf{w}_d$$

Determining the number of component

$$
\begin{aligned}
&(\mathbf{z}_i - \mathbf{z}_i^k)^T(\mathbf{z}_i - \mathbf{z}_i^k) = \\
&\left[(\mathbf{w}_{k+1}^T\mathbf{x}_i)\mathbf{w}_{k+1} + \ldots + (\mathbf{w}_d^T\mathbf{x}_i)\mathbf{w}_d\right]^T\left[(\mathbf{w}_{k+1}^T\mathbf{x}_i)\mathbf{w}_{k+1} + \ldots + (\mathbf{w}_d^T\mathbf{x}_i)\mathbf{w}_d\right] \\
&= \mathbf{w}_{k+1}^T(\mathbf{w}_{k+1}^T\mathbf{x}_i)^2\mathbf{w}_{k+1} + \ldots + \mathbf{w}_d^T(\mathbf{w}_d^T\mathbf{x}_i)^2\mathbf{w}_d \\
&(\text{note } \mathbf{w}_i^T\mathbf{w}_j = 0 \forall i \neq j \text{ since } \mathbf{w}_i \text{ and } \mathbf{w}_j \text{ are orthogonal vectors}) \\
&= (\mathbf{w}_{k+1}^T\mathbf{x}_i)^2\mathbf{w}_{k+1}^T\mathbf{w}_{k+1} + \ldots + (\mathbf{w}_d^T\mathbf{x}_i)^2\mathbf{w}_d^T\mathbf{w}_d \\
&= (\mathbf{w}_{k+1}^T\mathbf{x}_i)^2 + \ldots + (\mathbf{w}_d^T\mathbf{x}_i)^2 \\
&= (\mathbf{w}_{k+1}^T\mathbf{x}_i)(\mathbf{x}_i^T\mathbf{w}_{k+1}) + \ldots + (\mathbf{w}_d^T\mathbf{x}_i)(\mathbf{x}_i)^T\mathbf{w}_d \\
&= \mathbf{w}_{k+1}^T(\mathbf{x}_i\mathbf{x}_i^T)\mathbf{w}_{k+1} + \ldots + \mathbf{w}_d^T(\mathbf{x}_i\mathbf{x}_i^T)\mathbf{w}_d
\end{aligned}
$$

Determining the number of component

$$\frac{1}{N}\sum_{i=1}^{N}(\mathbf{z}_i - \mathbf{z}_i^k)^T(\mathbf{z}_i - \mathbf{z}_i^k) =$$

$$\frac{1}{N}\sum_{i=1}^{N}\left[\mathbf{w}_{k+1}^T(\mathbf{x}_i\mathbf{x}_i^T)\mathbf{w}_{k+1} + ... + \mathbf{w}_d^T(\mathbf{x}_i\mathbf{x}_i^T)\mathbf{w}_d\right]$$

$$= \mathbf{w}_{k+1}^T\left[\frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i\mathbf{x}_i^T)\right]\mathbf{w}_{k+1} + ... + \mathbf{w}_d^T\left[\frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i\mathbf{x}_i^T)\right]\mathbf{w}_d$$

$$= \mathbf{w}_{k+1}^T\Sigma\mathbf{w}_{k+1} + ... + \mathbf{w}_d^T\Sigma\mathbf{w}_d$$

(Note: $\Sigma\mathbf{w}_{k+1} = \lambda_{k+1}\mathbf{w}_{k+1}, ..., \Sigma\mathbf{w}_d = \lambda_d\mathbf{w}_d$)

$$= \mathbf{w}_{k+1}^T\lambda_{k+1}\mathbf{w}_{k+1} + \mathbf{w}_d^T\lambda_d\mathbf{w}_d$$

$$= \lambda_{k+1} + ... + \lambda_d$$

Determining the number of component

$$\frac{1}{N}\sum_{i=1}^{N}(\mathbf{z}_i - \mathbf{z}_i^k)^T(\mathbf{z}_i - \mathbf{z}_i^k) = \lambda_{k+1} + ... + \lambda_d$$

The mean square error of the truncated representation is equal to the sum of the remaining eigenvalues.

In general: choose k so that $90-95\%$ of the variance of the data is captured.

PCA - Advantages

- Optimal linear dimensionality reduction technique in the mean-square sense;
- Reduce the curse-of-dimensionality;
- Computational overhead of subsequent processing stages is reduced;
- Noise may be reduced;
- A projection into a subspace of a very low dimensionality, e.g. two dimensions, is useful for visualizing the data.

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