Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part VI

Three Models for Decision Problems

In increasing order of complexity

- Find a discriminant function $f(\mathbf{x})$ which maps each input directly onto a class label.
- Discriminative Models
  1.
  2.
- Generative Models
  1. Solve the inference problem of determining the class-conditional probabilities $p(\mathbf{x} \mid \mathcal{C}_k)$.
  2. *Also, infer the prior class probabilities*
  3. *Use Bayes theorem to find the posterior* $p(\mathcal{C}_k \mid \mathbf{x})$.
  4. Alternatively, model the joint distribution $p(\mathbf{x}, \mathcal{C}_k)$ directly.
  5. Use decision theory to assign each new $\mathbf{x}$ to one of the classes.

Data Generating Process

Given:

- class prior $p(\mathbf{t})$
- class-conditional $p(\mathbf{x} \mid \mathbf{t})$

to genera...

1. Sa...
2. Sa... distribution $p(\mathbf{x} \mid \mathbf{t})$.

(more about sampling later — this is called ...

Thinking about the data generating process is a usef... modelling step, especially when we have more prior knowledge.

Probabilistic Generative Models

- Generative approach: model class-conditional densities $p(\mathbf{x} \mid \mathcal{C}_k)$ and *class* priors (not parameter priors!) $p(\mathcal{C}_k)$ to calculate the posterior probability for class $\mathcal{C}_1$

$$p(\mathcal{C}_1 \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \mathcal{C}_1)p(\mathcal{C}_1)}{\quad}$$

where a and the logistic sigmoid function

$$a(\mathbf{x}) = \ln \frac{p(\mathbf{x} \mid \mathcal{C}_1)\, p(\mathcal{C}_1)}{p(\mathbf{x} \mid \mathcal{C}_2)\, p(\mathcal{C}_2)} = \ln \frac{\quad}{\quad}$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

- One point of this re-writing: we may learn $a(\mathbf{x})$ directly as *e.g.* a deep neural network.

Logistic Sigmoid

- The logistic sigmoid function is called a “squashing function” because it squashes the real axis into a finite interval $(0, 1)$.
- Well known properties (derive them):
  - Symmetry: $\sigma(\quad a) = 1 \quad\; \sigma(a)$
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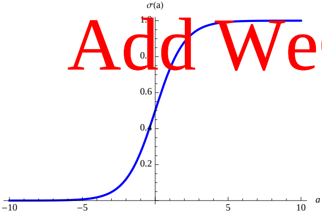
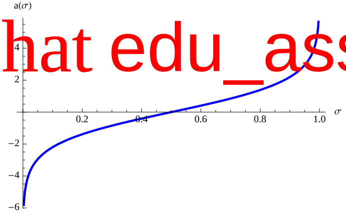


Sigmoid $\sigma(a) = \frac{1}{1+\exp(-a)}$



Logit $a(\sigma) = \ln\left(\frac{\sigma}{1-\sigma}\right)$

Probabilistic Generative Models - Multiclass

- The normalised exponential is given by

$$p(\mathcal{C}_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \mathcal{C}_k)\, p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} \mid \mathcal{C}_j)\, p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

wh

- Usually called the softmax function as it is a smoo version of the $\arg\max$ function, in particul

$$a_k \gg a_j \; \forall j \neq k \Rightarrow \Big(p(\mathcal{C}_k \mid \mathbf{x}) \approx 1 \wedge$$

- So, softargmax is a more descriptive though less common name.

- Assume class-conditional probabilities are Gaussian, with the same covariance and different mean:

- Let's characterise the posterior probabilities.
- We may separate the quadratic and linear term i

$$p(\mathbf{x} \mid \mathcal{C}_k)$$

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

$$= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}\mathbf{x}^T \boldsymbol{\Sigma}^{-1}\mathbf{x} + \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k\right\}$$

Probabil. Generative Model - Continuous Input

- For two classes

$$p(\mathcal{C}_1 \mid \mathbf{x}) = \sigma(a(\mathbf{x}))$$

and $a(\mathbf{x})$ is linear because the quadratic terms in $\mathbf{x}$ cancel (*c.f.* the previous slide):

$$\exp\left(\boldsymbol{\mu}_2^T \boldsymbol{\Sigma}^{-} \mathbf{x} - \tfrac{1}{2}\boldsymbol{\mu}_2^T \boldsymbol{\Sigma}^{-} \boldsymbol{\mu}\right) \qquad p(\ _2)$$

- Therefore

$$p(\mathcal{C}_1 \mid \mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x} + w$$

where

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

$$w_0 = -\frac{1}{2}\boldsymbol{\mu}_1^T\,\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T\,\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}$$

Probabil. Generative Model - Continuous Input

Class-conditional densities for two classes (left). Posterior probability $p(\mathcal{C}_1 \,|\, \mathbf{x})$ (right). Note the logistic sigmoid of a linear function of $\mathbf{x}$.

General Case - K Classes, Shared Covariance

- Use the normalised exponential

$$p(\mathcal{C}_k \,|\, \mathbf{x}) = \frac{p(\mathbf{x} \,|\, \mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} \,|\, \mathcal{C}_j)p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

wh

- to ge

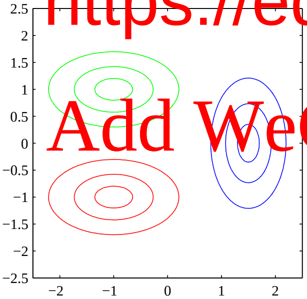
$$a_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}.$$

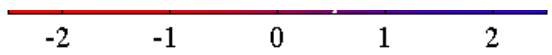
where

$$\mathbf{w}_k = \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_k$$
$$w_{k0} = -\frac{1}{2}\boldsymbol{\mu}_k^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_k + p(\mathcal{C}_k).$$

General Case - K Classes, Different Covariance

- If the class-conditional distributions have different covariances, the quadratic terms $-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}$ do not cancel out.
- We get a quadratic discriminant.





Parameter Estimation

- Given the functional form of the class-conditional densities $p(\mathbf{x} \mid \mathcal{C}_k)$, how can we determine the parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ and the class prior?

- Given the functional form of the class-conditional densities $p(\mathbf{x} \,|\, \mathcal{C}_k)$, how can we determine the parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ and the class prior?
- Simplest is maximum likelihood.
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cod
$t_n =$
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with the same covariance, but different mean.
- Denote the prior probability $p(\mathcal{C}_1) = \pi$, a
$p(\mathcal{C}_2) = 1 - \pi$.
- Then

$$p(\mathbf{x}_n, \mathcal{C}_1) = p(\mathcal{C}_1) p(\mathbf{x}_n \,|\, \mathcal{C}_1) = \pi \, \mathcal{N}(\mathbf{x}_n \,|\, \boldsymbol{\mu}_1, \boldsymbol{\Sigma})$$
$$p(\mathbf{x}_n, \mathcal{C}_2) = p(\mathcal{C}_2) p(\mathbf{x}_n \,|\, \mathcal{C}_2) = (1 - \pi) \, \mathcal{N}(\mathbf{x}_n \,|\, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

Maximum Likelihood Solution

- Thus the likelihood for the whole data set $\mathbf{X}$ and $\mathbf{t}$ is given by

$$p(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

$$= \prod_{n=1}^{N} [\pi \, \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma})]^{t_n} \, [(1-\pi) \, \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma})]^{1-t_n}$$

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- The t

$$\sum_{n=1}^{N} (t_n \ln \pi + (1-t_n) \ln(1$$

- which is maximal for (derive it)

$$\pi = \frac{1}{N} \sum_{n=1}^{N} t_n = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2}$$

where N_1 is the number of data points in class $\mathcal{C}_1$.

- Similarly, we can maximise the likelihood $p(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$ w.r.t. the means $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$, to get

$$\boldsymbol{\mu}_2 = \frac{1}{N_2} \sum_{n=1}^{N} (1 - t_n)$$

- For each class, this are the means of all input vect assigned to this class.

Maximum Likelihood Solution

- Finally, the log likelihood $\ln p(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$ can be ma

$$\mathbf{S}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n$$

Discrete Features - Naïve Bayes

- Assume the input space consists of discrete features, in the simplest case $x_i \in \{0, 1\}$.
- For a D-dimensional input space, a general distribution would be represented by a table with 2^D entries.
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ind
- Gro

- The Naïve Bayes assumption is that, given the class $\mathcal{C}_k$, the features are independent of each other:

$$
\begin{aligned}
p(\mathbf{x} \mid \mathcal{C}_k) &= \prod_{i=1}^{D} p(x_i \mid \mathcal{C}) \\
&= \prod_{i=1}^{D} \mu_{ki}^{x_i} (1 - \mu_{ki})^{1 - x_i}
\end{aligned}
$$

Discrete Features - Naïve Bayes

- With the naïve Bayes

$$p(\mathbf{x} \mid \mathcal{C}_k) = \prod_{i=1}^{D} \mu_{ki}^{x_i}(1 - \mu_{ki})^{1-x_i}$$

- we c exp

$$p(\mathcal{C}_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \mathcal{C}_k) p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} \mid \mathcal{C}_j) p(\mathcal{C}_j)} = \frac{\qquad}{\qquad}$$

- as a linear function of the x_i

$$a_k(\mathbf{x}) = \sum_{i=1}^{D} \{x_i \ln \mu_{ki} + (1 - x_i) \ln(1 - \mu_{ki})\} + \ln p(\mathcal{C}_k).$$

In increasing order of complexity

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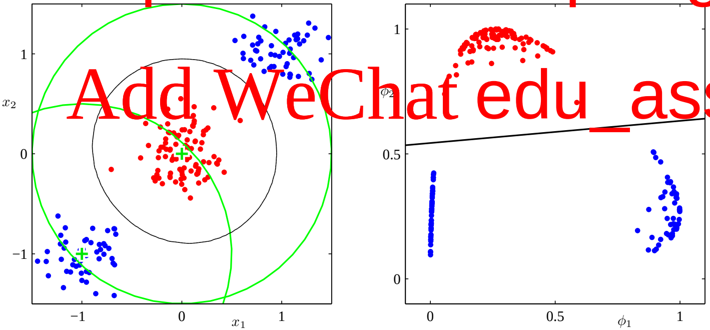
Probabilistic Discriminative Models

- Discriminative training: learn only to discriminate between the classes.
- Maximise a likelihood function defined through the conditional distribution $p(\mathcal{C}_k \mid \mathbf{x})$ directly.
- Ty
- As w be b class-conditional density assumptions $p(\mathbf{x} \mid \mathcal{C}_k)$ poorly approximate the true distributions.
- But: discriminative models can not create syn as $p(\mathbf{x})$ is not modelled.
- As an aside: *certain theoretical analyses show that generative models converge faster to their — albeit worse — asymptotic classification performance and are superior in some regimes.*

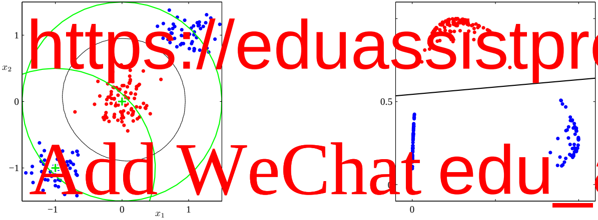
Original Input versus Feature Space

- So far in classification, we used direct input $\mathbf{x}$.
- All classification algorithms work also if we first apply a fixed nonlinear transformation of the inputs using a vector of basis functions $\phi(\mathbf{x})$.
- Example: Use two Gaussian basis functions centered at the g



Original Input versus Feature Space

- Linear decision boundaries in the feature space generally correspond to nonlinear boundaries in the input space.
- Classes which are NOT linearly separable in the input space may become linearly separable in the feature space:



- If classes overlap in input space, they will also overlap in feature space — nonlinear features $\phi(\mathbf{x})$ can not remove the overlap; but they may increase it.

Original Input versus Feature Space

- Fixed basis functions do not adapt to the data and therefore have important limitations (see discussion in Lin
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instead of the original input space.
- Some applications use fixed features succes avoiding the limitations

- We will therefore use ϕ instead of $\mathbf{x}$ fro

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Logistic Regression

- Two classes where the posterior of class $\mathcal{C}_1$ is a logistic sigmoid $\sigma()$ acting on a linear function of the input:

$$p(\mathcal{C}_1 \mid \phi) = y(\phi) = \sigma(\mathbf{w}^T \phi)$$

- $p(\mathcal{C}$
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- Compare this to fitting two Gaussians, which ha
quadratic number of parameters in M:

$$\underbrace{2M}_{\text{means}} + \underbrace{M(M+1)/2}_{\text{shared covariance}}$$

- For larger M, the logistic regression model has a clear advantage.

Logistic Regression

- Determine the parameter via maximum likelihood for data $(\phi_n, t_n), n = 1, \dots, N$, where $\phi_n = \phi(\mathbf{x}_n)$. The class membership is coded as $t_n \in \{0, 1\}$.
- Likelihood function

  where $y_n = p(\mathcal{C}_1 \mid \phi_n)$.
- Error function: negative log likelihood resulting in the cross-entropy error function

$$E(\mathbf{w}) = -\ln p(\mathbf{t} \mid \mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

- Error function (cross-entropy loss)

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

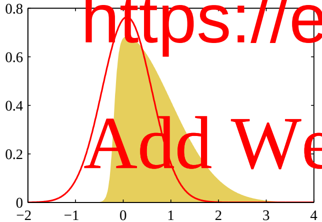
- y_n
- We
rule

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n)$$

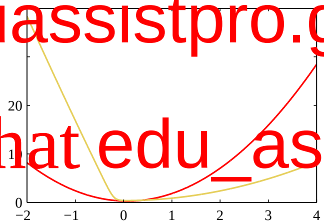
- for each data point error is product of deviation $y_n - t_n$ and basis function ϕ_n.
- We can now use gradient descent.
- We may easily modify this to reduce over-fitting by using regularised error or MAP (how?).

Laplace Approximation

- Given a continous distribution $p(x)$ which is not Gaussian, can we approximate it by a Gaussian $q(x)$?
- Need to find a mode of $p(x)$. Try to find a Gaussian with the same mode:



p.d.f. of :
Non-Gaussian (yellow) and
Gaussian approximation (red).



negative log p.d.f. of :
Non-Gaussian (yellow) and
Gaussian approxmation. (red).

Laplace Approximation

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- Cheap and nasty but sometimes effective.
- Assume $p(x)$ can be written as

$$p(z) = \frac{1}{Z} f(z)$$

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  app
- A mode of $p(z)$ is at a point z_0 where p'
- Taylor expansion of $\ln f(z)$ at z_0

$$\ln f(z) \simeq \ln f(z_0) - \frac{1}{2} A (z - z_0)^2$$

where

$$A = -\frac{d^2}{dz^2} \ln f(z) \mid_{z=z_0}$$

Laplace Approximation

- Exponentiating

$$\ln f(z) \simeq \ln f(z_0) - \frac{1}{2}A(z - z_0)^2$$

- we g

- And after normalisation we get the Laplace app

$$q(z) = \left(\frac{A}{2\pi}\right)^{1/2} \exp\{-\frac{A}{2}(z$$

- Only defined for precision $A > 0$ as only then $p(z)$ has a maximum.

Laplace Approximation - Vector Space

- Approximate p($\mathbf{z}$) for $z \in \mathbb{R}^M$

$$p(\mathbf{z}) = \frac{1}{Z} f(\mathbf{z})$$

- we get the Taylor expansion

- where the Hessian $\mathbf{A}$ is defined as

$$\mathbf{A} = -\nabla\nabla \ln f(\mathbf{z})\,|_{\mathbf{z}=\mathbf{z}_0}$$

- The Laplace approximation of $p(\mathbf{z})$ is th

$$q(\mathbf{z}) \propto \exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^T \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\}$$

$$\Rightarrow q(\mathbf{z}) = \mathcal{N}(\mathbf{z}\,|\,\mathbf{z}_0, \mathbf{A}^{-1})$$

- Exact Bayesian inference for the logistic regression is intractable.
- Wh and l sig

- Eva
- Therefore we will use the Laplace approximati
- The predictive distribution remains intractabl the Laplace approximation to the posterior dis it can be approximated.

- Assume a Gaussian prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_0, \mathbf{S}_0)$$

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- For a set of training data $(\mathbf{x}_n, t_n)$, where
posterior is given by

$$p(\mathbf{w} \mid \mathbf{t}) \propto p(\mathbf{w}) p(\mathbf{t} \mid \mathbf{w}$$

where $\mathbf{t} = (t_1, \dots, t_N)^T$.

- Using our previous result for the cross-entropy function

$$E(\mathbf{w}) = -\ln p(\mathbf{t} \,|\, \mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

we c

using the notation $y_n = \sigma(\mathbf{w}^T \phi_n)$ as

$$\ln p(\mathbf{w} \,|\, \mathbf{t}) = -\frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^T \mathbf{S}_0^{-1} (\mathbf{w}$$

$$+ \sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

- To obtain a Gaussian approximation to

$$\ln p(\mathbf{w} \mid \mathbf{t})$$

$$= -\frac{1}{2}(\mathbf{w} - \mathbf{m}_0)^T \mathbf{S}_0^{-1}(\mathbf{w} - \mathbf{m}_0) + \sum^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

1. nonlinear function in $\mathbf{w}$ because $y_n = \quad ^T$
2. *Calculate the second derivative of the negati to get the inverse covariance of the Laplace ap*

$$\mathbf{S}_N = -\nabla\nabla \ln p(\mathbf{w} \mid \mathbf{t}) = \mathbf{S}_0^{-1} + \sum_{n=1}^{N} \quad {}_n \quad - \quad {}_n \quad {}_n \quad {}_n$$

Nowadays the gradient and Hessian would be computed with automatic differentiation; one need only implement $\ln p(\mathbf{w} \mid \mathbf{t})$.

Bayesian Logistic Regression

- The approximated Gaussian (via Laplace approximation) of the posterior distribution is now

wh

$$\mathbf{S}_N = -\nabla\nabla \ln p(\mathbf{w} \mid \mathbf{t}) = \mathbf{S}_0^{-1} + \sum_{n=1}^{N}$$