Probabilistic Machine Learning

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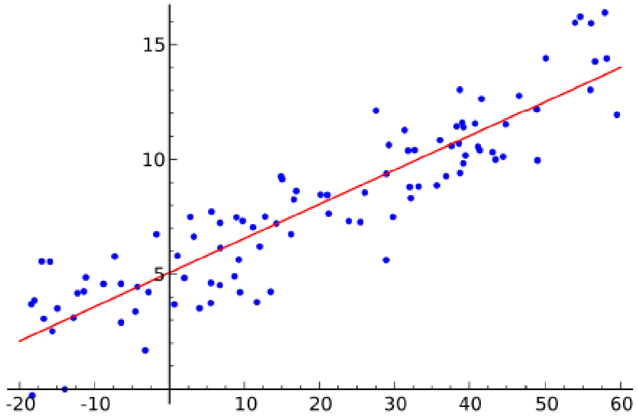
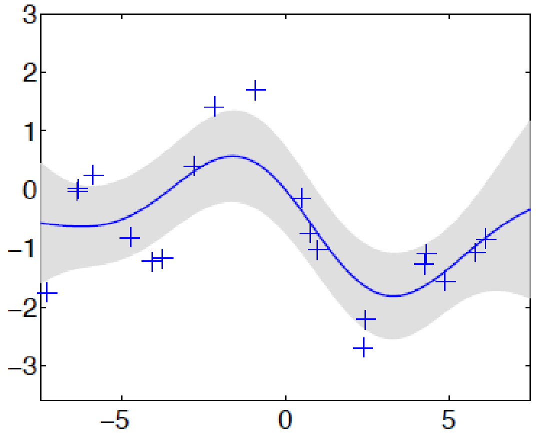
Outline

- *Probabilistic* Linear Regression
- *Probabilistic* Classification
- *Probabilistic* Clustering
- *Probabilistic* Dimension Reduction

Probabilistic Linear Regression

$$P(X \mid \theta) = \text{Probability [data} \mid \text{pattern]}$$





- Inference idea

data = underlying pattern + independent noise

- Change your viewpoint of data
  - Generative model

Probabilistic Linear Regression

- Each response generated by a linear model plus Gaussian noise

$$y = \omega^T x + \varepsilon, \quad \varepsilon \sim \mathcal{N}\left(0, \sigma^2\right)$$

- Each response y then becomes a draw from the following Gaussian:

$$y \sim \left(\omega^T x, \sigma^2\right)$$

- Probability of each response variable

$$P(y \mid x, \omega) = \mathcal{N}\left(\omega^T x, \sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}\left(y - \omega^T x\right)^2\right)$$

- Given observed data $D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_m, y_m)\}$, we want to estimate the weight vector ω

Maximum Likelihood Estimation

- Log-likelihood:

$$
\begin{aligned}
\ell(\omega) = \log L(\omega) &= \log P(D \mid \omega) \\
&= \log P(Y \mid X, \omega) \\
&= \log \prod_{n=1}^{m} P\left(y_n \mid x_n, \omega\right) \\
&= \sum_{n=1}^{m} \log P\left(y_n \mid x_n, \omega\right) \\
&= \sum_{n=1}^{m} \log \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\left(y_n - \omega^T x_n\right)^2}{2\sigma^2}\right) \\
&= \sum_{n=1}^{m} \left\{-\frac{1}{2}\log\left(2\pi\sigma^2\right) - \frac{\left(y_n - \omega^T x_n\right)^2}{2\sigma^2}\right\}
\end{aligned}
$$

Maximum Likelihood Estimation

- Maximum Likelihood Solution:

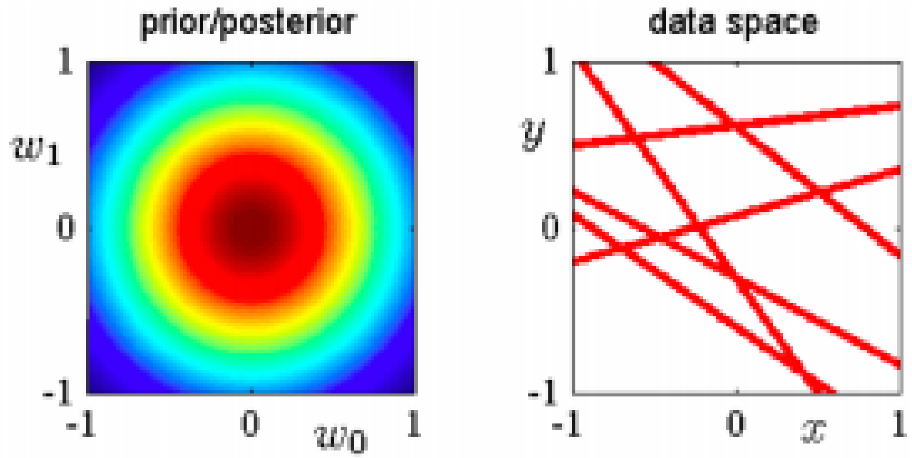
$$
\begin{aligned}
\hat{\omega}_{MLE} &= \arg\max_{\omega} \log P(D \mid \omega) \\
&= \arg\max_{\omega} \; -\frac{1}{2\sigma^2} \sum_{n=1}^{m} \left(y_n - \omega^T x_n\right)^2 \\
&= \arg\min_{\omega} \frac{1}{2\sigma^2} \sum_{n=1}^{m} \left(y_n - \omega^T x_n\right)^2 \\
&= \arg\min_{\omega} \sum_{n=1}^{m} \left(y_n - \omega^T x_n\right)^2
\end{aligned}
$$

- It is equivalent to the least-squares objective for linear regression (amazing !)
- In least squares, we implicitly assume that noise is Gaussian distributed

Maximum-a-Posteriori Solution

- Let's assume a Gaussian prior distribution over the weight vector ω
  - (Make sure you understand what it means)

$$P(\omega) \sim \mathcal{N}\left(\omega \mid \underline{0, \lambda^{-1} I}\right) = \frac{1}{(2\pi)^{D/2}} \exp\left(-\frac{\lambda}{2}\omega^T \omega\right)$$



- Log posterior probability:

$$\log P(\omega \mid D) = \log \frac{P(\omega)P(D \mid \omega)}{P(D)} = \log P(\omega) + \log P(D \mid \omega) - \underbrace{\log P(D)}_{\text{constant}}$$

Maximum-a-Posteriori Solution

- Maximum-a-Posteriori Solution:

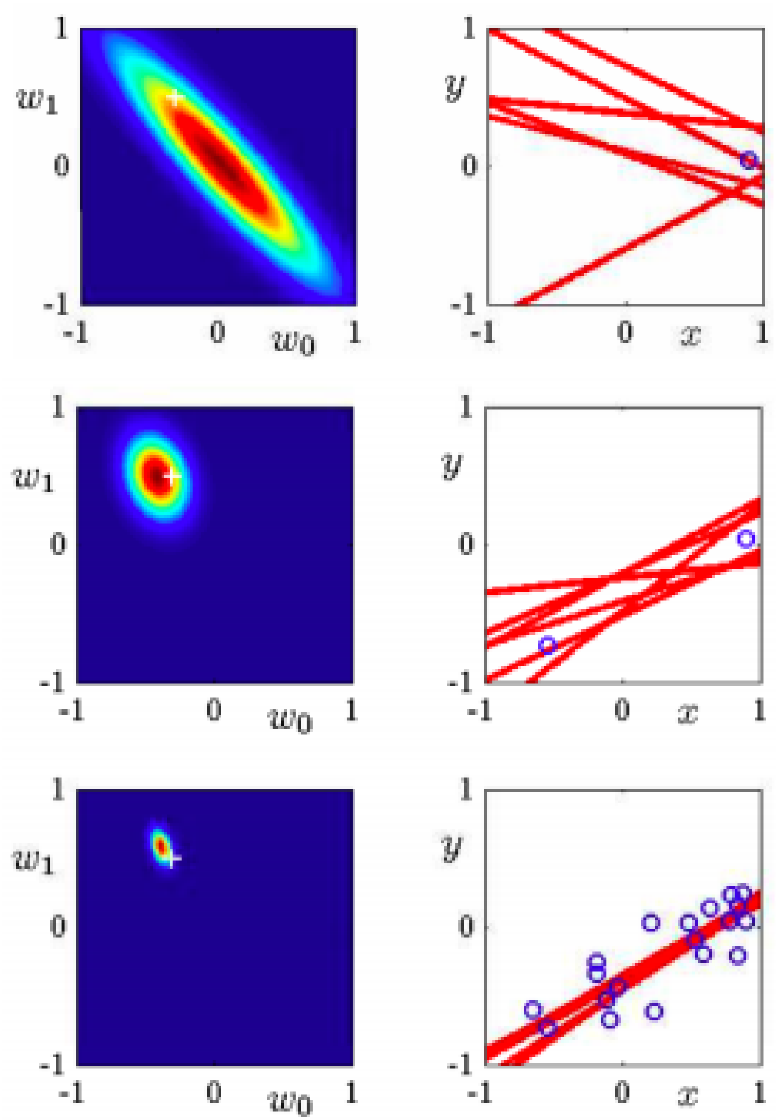
$$
\begin{aligned}
&\hat{\omega}_{MAP} \\
&= \arg\max_{\omega} \log P(\omega \mid D) \\
&= \arg\max_{\omega} \{\log P(\omega) + \log P(D \mid \omega)\} \\
&= \arg\max_{\omega} \left\{ -\frac{D}{2}\log(2\pi) - \frac{\lambda}{2}\omega^T\omega + \sum_{n=1}^{m}\left\{ -\frac{1}{2}\log\left(2\pi\sigma^2\right) - \frac{\left(y_n - \omega^T x_n\right)^2}{2\sigma^2} \right\} \right\} \\
&= \arg\min_{\omega} \frac{1}{2\sigma^2}\sum_{n=1}^{m}\left(y_n - \omega^T x_n\right)^2 + \frac{\lambda}{2}\omega^T\omega \\
&\text{(ignoring constants and changing max to min)}
\end{aligned}
$$

- For $\sigma = 1$ (or some constant) for each input, it's equivalent to the regularized least-squares objective (amazing !)

- Big lesson: MAP = l_2 norm regularization

MAP Illustration

- One observation
- Two observations
- 20 observations



Summary: MLE vs MAP

- MLE solution:

$$\hat{\omega}_{MLE} = \arg\min_{\omega} \frac{1}{2\sigma^2} \sum_{n=1}^{m} \left(y_n - \omega^T x_n\right)^2$$

- MAP solution:

$$\hat{\omega}_{MLE} = \arg\min_{\omega} \frac{1}{2\sigma^2} \sum_{n=1}^{m} \left(y_n - \omega^T x_n\right)^2 + \frac{\lambda}{2}\omega^T \omega$$

- Take-home messages:
  - MLE estimation of a parameter leads to unregularized solutions
  - MAP estimation of a parameter leads to regularized solutions
  - The prior distribution acts as a regularizer in MAP estimation

- Note : for MAP, different prior distributions lead to different regularizers
  - Gaussian prior on ω regularizes the l_2 norm of ω
  - Laplace prior $exp(-C\|\omega\|_1)$ on ω regularizes the l_1 norm of ω

Probabilistic Linear Classification

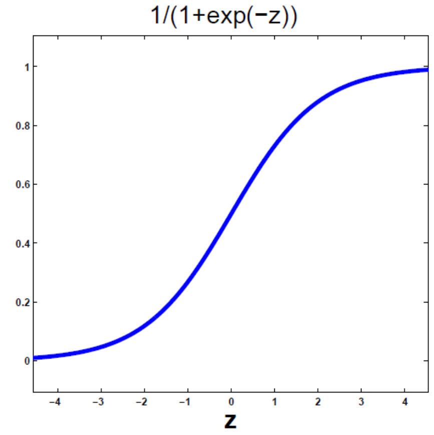
- Andrew Ng. lecture on GDA (generative model)
- Lecture note in pdf and video on YouTube (https://see.stanford.edu/Course/CS229/50)

- http://cs229.stanford.edu/syllabus.html

Probabilistic Linear Classification

- Often we do not just care about predicting the label y for an example
- Rather, we want to predict the label probabilities
  - E.g., $P(y=+1|\ x,\omega)$: the probability that the label is $P(y|x,\omega)$
  - In a sense, it is our confidence in the predicted label $+1$
- Probabilistic classification models allow us do that $(y=-1/+1)$
- Consider the following function in a compact expression

$$P(y \mid x, \omega) = \sigma\left(y\omega^T x\right) = \frac{1}{1+\exp(-y\omega^T x)}$$

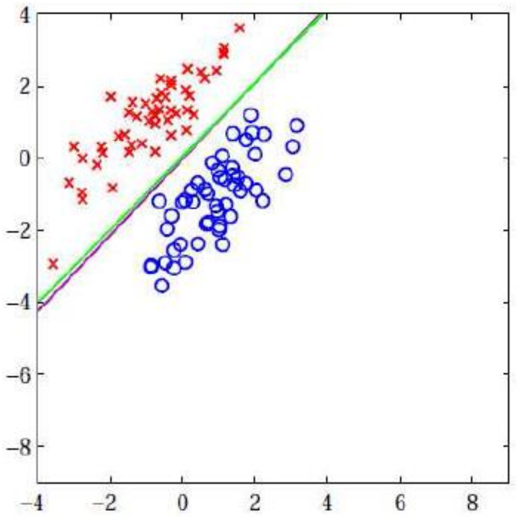


- σ is the logistic function which maps all real number into $(0,1)$

Logistic Regression

- What does the decision boundary look like for logistic regression?
- At the decision boundary labels $-1/+1$ becomes equiprobable

$$
\begin{aligned}
P(y=+1 \mid x, \omega) &= P(y=-1 \mid x, \omega) \\
\frac{1}{1+\exp(-\omega^T x)} &= \frac{1}{1+\exp(\omega^T x)} \\
\exp\left(-\omega^T x\right) &= \exp\left(\omega^T x\right) \\
\omega^T x &= 0
\end{aligned}
$$



- The decision boundary is therefore linear

  $\Longrightarrow$ logistic regression is a linear classifier

- Note: it is possible to kernelize and make it nonlinear

Maximum Likelihood Solution

- Goal: want to estimate ω from the data $D = \{(x_1, y_1), \cdots, (x_m, y_m)\}$
- Log-likelihood:

$$
\begin{aligned}
\ell(\omega) = \log L(\omega) &= \log P(D \mid \omega) \\
&= \log P(Y \mid X, \omega) \\
&= \log \prod_{n=1}^{m} P(y_n \mid x_n, \omega) \\
&= \sum_{n=1}^{m} \log P(y_n \mid x_n, \omega) \\
&= \sum_{n=1}^{m} \log \frac{1}{1 + \exp(-y_n \omega^T x_n)} \\
&= \sum_{n=1}^{m} -\log\left[1 + \exp\left(-y_n \omega^T x_n\right)\right]
\end{aligned}
$$

Maximum Likelihood Solution

- Maximum Likelihood Solution:

$$\hat{\omega}_{MLE} = \arg\max_{\omega} \log L(\omega) = \arg\min_{\omega} \sum_{n=1}^{m} \log\left[1 + \exp\left(-y_n \omega^T x_n\right)\right]$$

- No closed-form solution exists, but we can do
  - CVXPY (we did it)
  - Gradient descent on ω

$$\begin{aligned}\nabla_{\omega} \log L(\omega) &= \sum_{n=1}^{m} -\frac{1}{1 + \exp(-y_n \omega^T x_n)} \exp\left(-y_n \omega^T x_n\right)\left(-y_n x_n\right) \\ &= \sum_{n=1}^{m} \frac{1}{1 + \exp\left(y_n \omega^T x_n\right)} y_n x_n\end{aligned}$$

Maximum-a-Posteriori Solution

- Let's assume a Gaussian prior distribution over the weight vector ω

$$P(\omega) = \mathcal{N}\left(\omega \mid 0, \lambda^{-1} I\right) = \frac{1}{(2\pi)^{D/2}} \exp\left(-\frac{\lambda}{2}\omega^T \omega\right)$$

- Maximum-a-Posteriori Solution:

$$\begin{aligned}
&\hat{\omega}_{MAP} \\
&= \arg\max_{\omega} \log P(\omega \mid D) \\
&= \arg\max_{\omega} \{\log P(\omega) + \log P(D \mid \omega) - \underbrace{\log P(D)}_{\text{constant}}\} \\
&= \arg\max_{\omega} \{\log P(\omega) + \log P(D \mid \omega)\} \\
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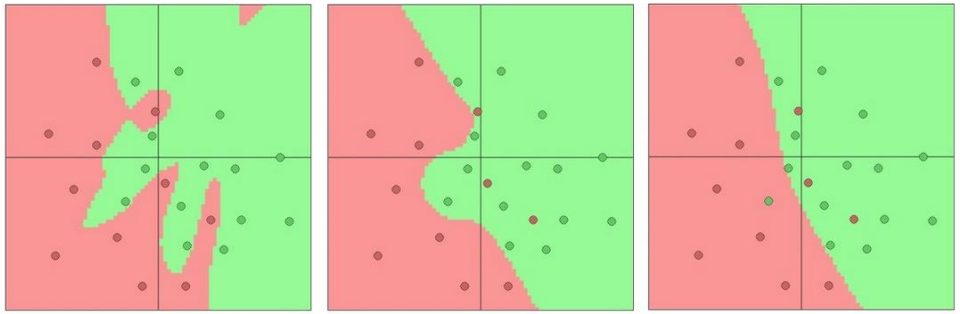
&= \arg\min_{\omega} \sum_{n=1}^{m} \log\left[1 + \exp\left(-y_n \omega^T x_n\right)\right] + \frac{\lambda}{2}\omega^T\omega \\
&\text{(ignoring constants and changing max to min)}
\end{aligned}$$

- Big lesson: MAP = l_2 norm regularization

Maximum-a-Posteriori Solution

- Q: What does regularizer do in a classifier?
- A: Nonlinear classifier gives more intuitive explanation



- No closed-form solution exists but we can do gradient descent on ω
  - See "A comparison of numerical optimizers for logistic regression" by Tom Minka on optimization techniques (gradient descent and others) for logistic regression
  - (both MLE and MAP)

Summary: MLE vs MAP

- MLE solution:

$$\hat{\omega}_{MLE} = \arg\min_{\omega} \sum_{n=1}^{m} \log\left[1 + \exp\left(-y\omega^T x_n\right)\right]$$

- MAP solution:

$$\hat{\omega}_{MAP} = \arg\min_{\omega} \sum_{n=1}^{m} \log\left[1 + \exp\left(-y\omega^T x_n\right)\right] + \frac{\lambda}{2}\omega^T \omega$$

- Take-home messages (we already saw these before)
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- Note: For MAP, different prior distributions lead to different regularizers
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Probabilistic Clustering

- will not cover in this course

Probabilistic Dimension Reduction

- will not cover in this course