IAML: Linear Regression

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Semester 1

Overview

- The linear model
- Fitting the linear model to data
- Probabilistic interpretation of the error function
- Examples of regression problems
- Dealing with multiple outputs
- Generalized linear regression
- Radial basis function (RBF) models

The Regression Problem

- Classification and regression problems:
  - Classification: target of prediction is discrete
  - Regression: target of prediction is continuous

- Training data: Set $\mathcal{D}$ of pairs $(\mathbf{x}_i, y_i)$ for $i = 1, \ldots, n$, where $\mathbf{x}_i \in \mathbb{R}^D$ and $y_i \in \mathbb{R}$
- Today: Linear regression, i.e., relationship between $\mathbf{x}$ and y is linear.
- Although this is simple (and limited) it is:
  - More powerful than you would expect
  - The basis for more complex nonlinear methods
  - Teaches a lot about regression and classification

Examples of regression problems

- Robot inverse dynamics: predicting what torques are needed to drive a robot arm along a given trajectory
- Electricity load forecasting, generate hourly forecasts two days in advance (see W & F, §1.3)
- Predicting staffing requirements at help desks based on historical data and product and sales information,
- Predicting the time to failure of equipment based on utilization and environmental conditions

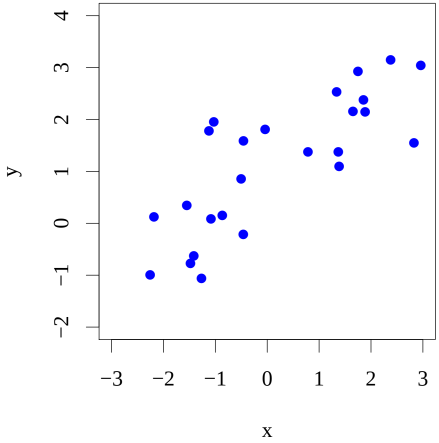
The Linear Model

- Linear model

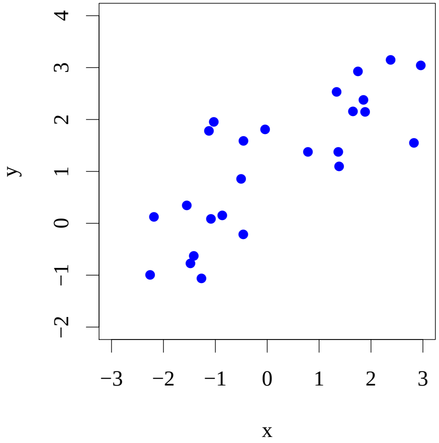
$$\begin{aligned} f(\mathbf{x};\mathbf{w}) &= w_0 + w_1 x_1 + \ldots + w_D x_D \\ &= \mathbf{w}^T \phi(\mathbf{x}) \end{aligned}$$

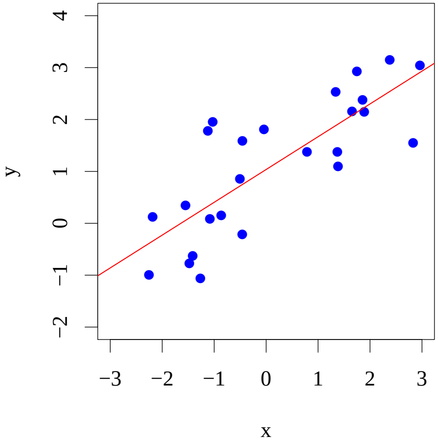
  where $\phi(\mathbf{x}) = (1, x_1, \ldots, x_D)^T = (1, \mathbf{x}^T)^T$
- The maths of fitting linear models to data is easy. We use the notation $\phi(\mathbf{x})$ to make generalisation easy later.

Toy example: Data

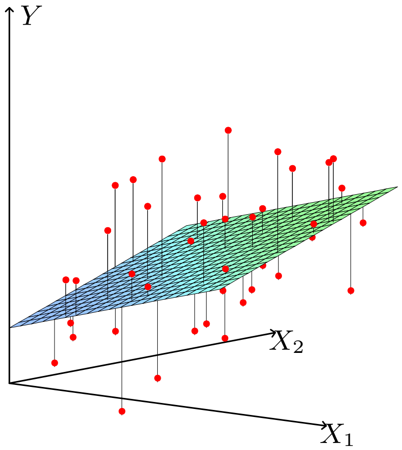


Toy example: Data





With two features



Instead of a line, a *plane*. With more features, a *hyperplane*.

Figure: Hastie, Tibshirani, and Friedman

With more features

CPU Performance Data Set

- Predict: PRP: published relative performance
- MYCT: machine cycle time in nanoseconds (integer)
- MMIN: minimum main memory in kilobytes (integer)
- MMAX: maximum main memory in kilobytes (integer)
- CACH: cache memory in kilobytes (integer)
- CHMIN: minimum channels in units (integer)
- CHMAX: maximum channels in units (integer)

With more features

```
PRP = - 56.1
      + 0.049 MYCT
      + 0.015 MMIN
      + 0.006 MMAX
      + 0.630 CACH
      - 0.270 CHMIN
      + 1.46 CHMAX
```

In matrix notation

- Design matrix is $n \times (D+1)$

$$\Phi = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1D} \\ 1 & x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nD} \end{pmatrix}$$

- x_{ij} is the jth component of the training input $\mathbf{x}_i$
- Let $\mathbf{y} = (y_1, \dots, y_n)^T$
- Then $\hat{\mathbf{y}} = \Phi \mathbf{w}$ is ...?

Linear Algebra: The 1-Slide Version

What is matrix multiplication?

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

First consider matrix times vector, i.e., $A\mathbf{b}$. Two answers:

1. $A\mathbf{b}$ is a linear combination of the columns of A

$$Ab = b_1 \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} + b_2 \begin{pmatrix} a_{12} \\ a_{22} \\ a_{32} \end{pmatrix} + b_3 \begin{pmatrix} a_{13} \\ a_{23} \\ a_{33} \end{pmatrix}$$

2. Ab is a vector. Each element of the vector is the dot products between b and *one row* of A.

$$A\mathbf{b} = \begin{pmatrix} (a_{11}, a_{12}, a_{13})\mathbf{b} \\ (a_{21}, a_{22}, a_{23})\mathbf{b} \\ (a_{31}, a_{32}, a_{33})\mathbf{b} \end{pmatrix}$$

Linear model (part 2)

In matrix notation:

- Design matrix is $n \times (D+1)$

$$\Phi = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1D} \\ 1 & x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nD} \end{pmatrix}$$

- x_{ij} is the jth component of the training input $\mathbf{x}_i$
- Let $\mathbf{y} = (y_1, \dots, y_n)^T$
- Then $\hat{\mathbf{y}} = \Phi \mathbf{w}$ is the model's predicted values on training inputs.

Solving for Model Parameters

This looks like what we've seen in linear algebra

$$\mathbf{y} = \Phi \mathbf{w}$$

We know $\mathbf{y}$ and Φ but not $\mathbf{w}$.

So why not take $\mathbf{w} = \Phi^{-1}\mathbf{y}$? (You can't, but why?)

Solving for Model Parameters

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We know **y** and Φ but not **w**.

So why not take $\mathbf{w} = \Phi^{-1}\mathbf{y}$? (You can't, but why?)

Three reasons:

- Φ is not square. It is $n \times (D+1)$.
- The system is overconstrained (n equations for $D+1$ parameters), in other words
- The data has noise

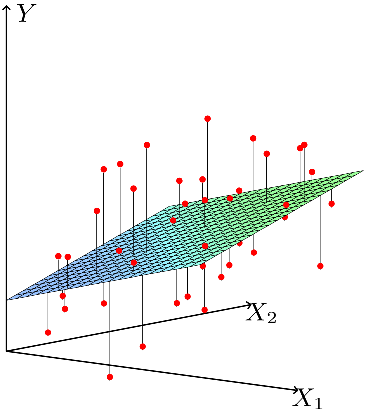
Loss function

Want a *loss function* $O(\mathbf{w})$ that

- We minimize wrt $\mathbf{w}$.
- At minimum, $\hat{\mathbf{y}}$ looks like $\mathbf{y}$.
- (Recall: $\hat{\mathbf{y}}$ depends on $\mathbf{w}$)

$$\hat{\mathbf{y}} = \Phi \mathbf{w}$$

Fitting a linear model to data



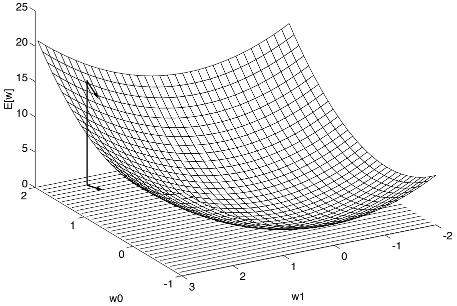
- A common choice: *squared error* (makes the maths easy)

$$O(\mathbf{w}) = \sum_{i=1}^{n} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

- In the picture: this is sum of squared length of black sticks.
- (Each one is called a *residual*, i.e., each $y_i - \mathbf{w}^T \mathbf{x}_i$)

Fitting a linear model to data

- $$O(\mathbf{w}) = \sum_{i=1}^{n} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$
  $$= (\mathbf{y} - \Phi\mathbf{w})^T (\mathbf{y} - \Phi\mathbf{w})$$
- We want to minimize this with respect to **w.**
- The error surface is a parabolic bowl



- How do we do this?

The Solution

- Answer: to minimize $O(\mathbf{w}) = \sum_{i=1}^{n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2$, set partial derivatives to 0.
- This has an analytical solution

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

- $(\Phi^T\Phi)^{-1}\Phi^T$ is the pseudo-inverse of Φ
- First check: Does this make sense? Do the matrix dimensions line up?
- Then: Why is this called a pseudo-inverse? ()
- Finally: What happens if there is one feature? No features?

Probabilistic interpretation of $O(\mathbf{w})$

- Assume that $y = \mathbf{w}^T\mathbf{x} + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$
- (This is an exact linear relationship plus Gaussian noise.)
- This implies that $y|\mathbf{x}_i \sim N(\mathbf{w}^T\mathbf{x}_i, \sigma^2)$, i.e.

$$-\log p(y_i|\mathbf{x}_i) = \log\sqrt{2\pi} + \log\sigma + \frac{(y_i - \mathbf{w}^T\mathbf{x}_i)^2}{2\sigma^2}$$

- So minimising $O(\mathbf{w})$ equivalent to maximising likelihood!
- Can view $\mathbf{w}^T\mathbf{x}$ as $E[y|\mathbf{x}]$.
- Squared residuals allow estimation of σ^2

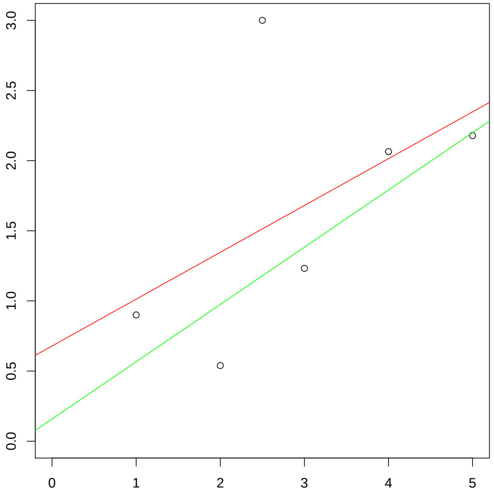
$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2$$

Fitting this into the general structure for learning algorithms:

- Define the **task**: regression
- Decide on the **model structure**: linear regression model
- Decide on the **score function**: squared error (likelihood)
- Decide on **optimization/search method** to optimize the score function: calculus (analytic solution)

Sensitivity to Outliers

- Linear regression is sensitive to *outliers*
- Example: Suppose $y = 0.5x + \epsilon$, where $\epsilon \sim N(0, \sqrt{0.25})$, and then add a point (2.5,3):



Diagnositics

Graphical diagnostics can be useful for checking:

- Is the relationship obviously nonlinear? Look for structure in residuals?
- Are there obvious outliers?

The goal isn't to find all problems. You can't. The goal is to find obvious, embarrassing problems.

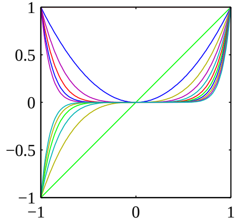
Examples: Plot residuals by fitted values. Stats packages will do this for you.

Dealing with multiple outputs

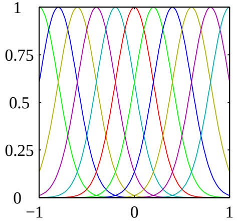
- Suppose there are q different targets for each input $\mathbf{x}$
- We introduce a different $\mathbf{w}_i$ for each target dimension, and do regression separately for each one
- This is called *multiple regression*

Basis expansion

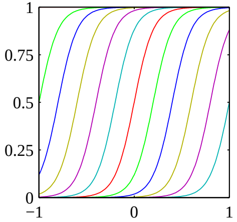
- We can easily transform the original attributes $\mathbf{x}$ non-linearly into $\phi(\mathbf{x})$ and do linear regression on them



polynomial



Gaussians



sigmoids

Figure credit: Chris Bishop, PRML

- Design matrix is $n \times m$

$$\Phi = \begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \dots & \phi_m(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \dots & \phi_m(\mathbf{x}_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(\mathbf{x}_n) & \phi_2(\mathbf{x}_n) & \dots & \phi_m(\mathbf{x}_n) \end{pmatrix}$$

- Let $\mathbf{y} = (y_1, \dots, y_n)^T$
- Minimize $E(\mathbf{w}) = |\mathbf{y} - \Phi\mathbf{w}|^2$. As before we have an analytical solution

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

- $(\Phi^T\Phi)^{-1}\Phi^T$ is the pseudo-inverse of Φ

Example: polynomial regression

$$\phi(x) = (1,\ x,\ x^2, \ldots, x^M)^T$$

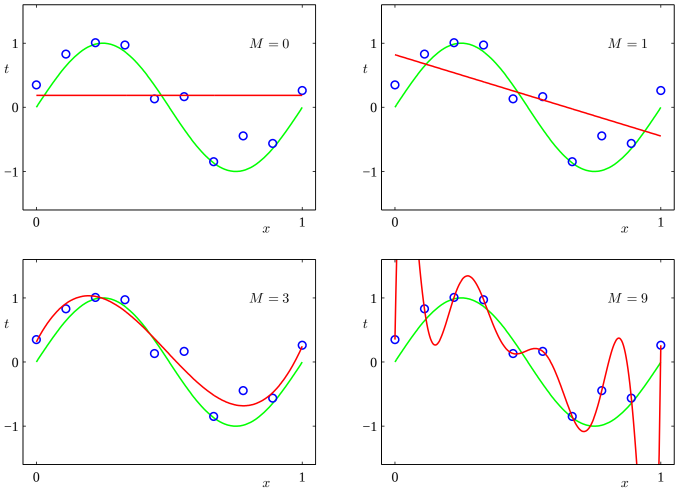


Figure credit: Chris Bishop, PRML

More about the features

- Transforming the features can be important.
- Example: Suppose I want to predict the CPU performance.
- Maybe one the features is *manufacturer*.

$$x_1 = \begin{cases} 1 & \text{if Intel} \\ 2 & \text{if AMD} \\ 3 & \text{if Apple} \\ 4 & \text{if Motorola} \end{cases}$$

- Let's use this as a feature. Will this work?

More about the features

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- Let's use this as a feature. Will this work?
- Not the way you want. Do you really believe AMD is double Intel?

More about the features

- Instead convert this into 0/1

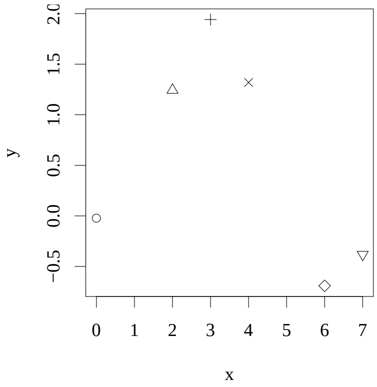
$$\begin{aligned} x_1 &= 1 \text{ if Intel, 0 otherwise} \\ x_2 &= 1 \text{ if AMD, 0 otherwise} \\ &\vdots \end{aligned}$$

- Note this is a consequence of linearity. We saw something similar with text in the first week.
- Other good transformations: log, square, square root

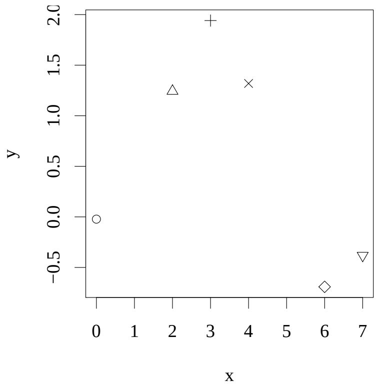
Radial basis function (RBF) models

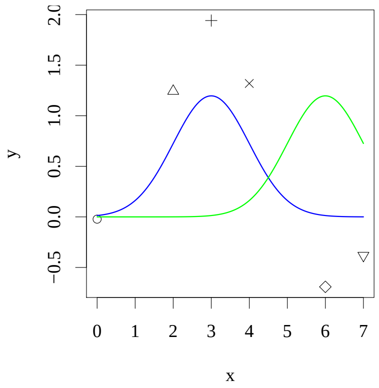
- Set $\phi_i(\mathbf{x}) = \exp(-\frac{1}{2}|\mathbf{x} - \mathbf{c}_i|^2/\alpha^2)$.
- Need to position these “basis functions” at some prior chosen centres $\mathbf{c}_i$ and with a given width α. There are many ways to do this but choosing a subset of the datapoints as centres is one method that is quite effective
- Finding the weights is the same as ever: the pseudo-inverse solution.

RBF example

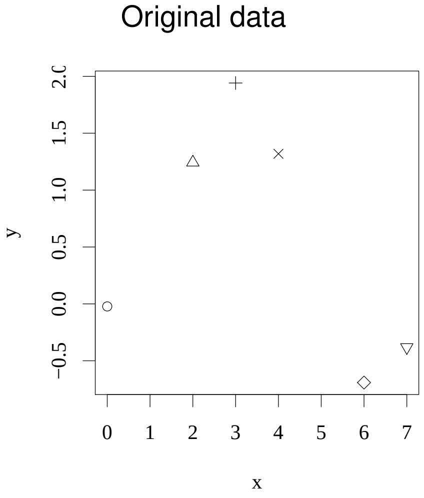


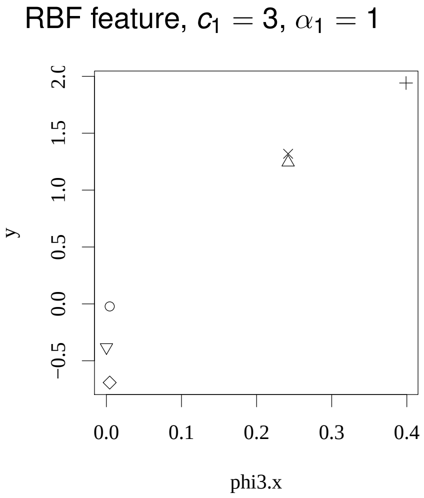
RBF example





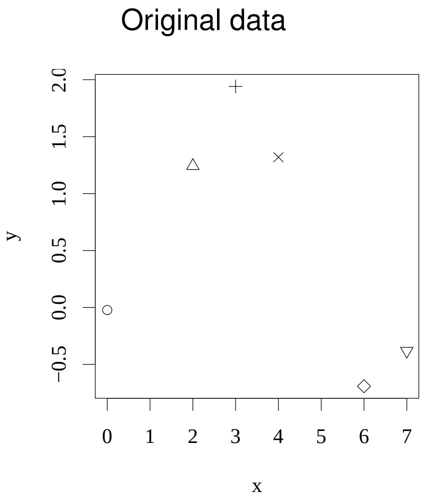
An RBF feature

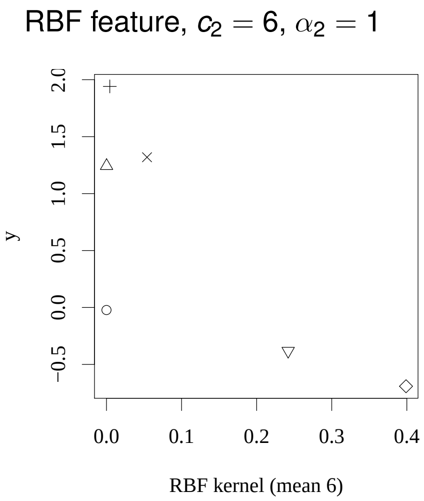




Another RBF feature

Notice how the feature functions “specialize” in input space.



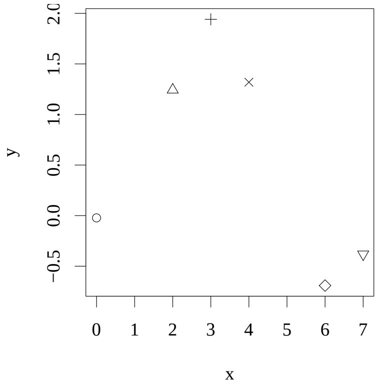


RBF example

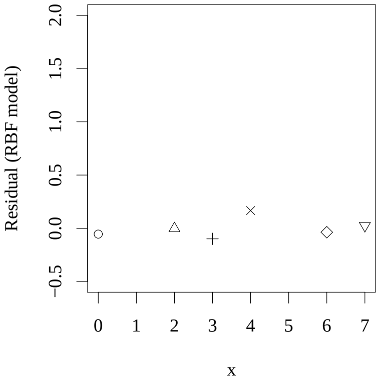
Run the RBF with both basis functions above, plot the residuals

$$y_i - \phi(\mathbf{x}_i)^T \mathbf{w}$$

Original data



Residuals



RBF: Ay, there’s the rub

- So why not use RBFs for everything?
- Short answer: You might need too many basis functions.
- This is especially true in high dimensions (we’ll say more later)
- Too many means you probably overfit.
- Extreme example: Centre one on each training point.
- Also: notice that we haven’t seen yet in the course how to learn the RBF *parameters*, i.e., the mean and standard deviation of each kernel
- Main point of presenting RBFs now: Set up later methods like support vector machines

Summary

- Linear regression often useful out of the box.
- More useful than it would be seem because linear means linear *in the parameters*. You can do a nonlinear transform of the data first, e.g., polynomial, RBF. This point will come up again.
- Maximum likelihood solution is computationally efficient (pseudo-inverse)
- Danger of overfitting, especially with many features or basis functions