22 Function learning algorithms

Important general learning problem:

Learning a function from examples

- Given a finite set of training pairs $(\mathbf{x}_1, y_1)$, $(\mathbf{x}_2, y_2)$, $\ldots$, $(\mathbf{x}_t, y_t)$
- Attempt to learn a rule for predicting y given $\mathbf{x}$

$$\begin{array}{c} \mathbf{x}_1, y_1 \\ \mathbf{x}_2, y_2 \\ \vdots \\ \mathbf{x}_t, y_t \end{array} \quad \Rightarrow \quad \boxed{\text{Learner}} \quad \Rightarrow \quad h : X \to Y$$

- Want to minimize prediction error, $\text{err}(h(x), y)$, on test examples (x, y)
- The function $\text{err}(\hat{y}, y)$ depends on the problem

  For *classification* problems, use

$$\text{err}(\hat{y}, y) = \begin{cases} 0 & \hat{y} = y \\ 1 & \hat{y} \neq y \end{cases}$$

  For *real-valued* prediction (regression) problems, use

$$\text{err}(\hat{y}, y) = (\hat{y} - y)^2$$

Generic learning algorithm

1. Fix a hypothesis space $H = \{\text{set of } h\text{'s}\}$
2. Given $(x_1, y_1) \ldots (x_t, y_t)$, calculate $h^* \in H$ that minimizes

$$\frac{1}{t} \sum_{i=1}^{t} \text{err}(h(x_i), y_i)$$

(average training error)

22.1 Special case: real valued prediction

Learn $h : \Re^n \rightarrow \Re$ to minimize the prediction error

$$\text{err}(\hat{y}, y) \;=\; (\hat{y} - y)^2$$

Assume

$$\begin{aligned} H &= \{\text{linear functions}\} \\ &= \{h_{\mathbf{w}} : \mathbf{w} \in \Re^n\} \\ &\quad \text{where } \; h_{\mathbf{w}}(\mathbf{x}) \;=\; \mathbf{w} \cdot \mathbf{x} \;=\; \textstyle\sum_{i=1}^n w_i x_i \end{aligned}$$

Given training data

$$\left[\begin{array}{cccc|c} x_{11} & x_{12} & \dots & x_{1n} & y_1 \\ x_{21} & x_{22} & \dots & x_{2n} & y_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{t1} & x_{t2} & \dots & x_{tn} & y_t \end{array}\right]$$

Calculate $\mathbf{w}$ that minimizes

$$SSE \;=\; \sum_{i=1}^t (\mathbf{w} \cdot \mathbf{x}_i - y_i)^2$$

$$\text{where } \; \mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{in})$$

Can solve for this $\mathbf{w}$ by taking derivatives of SSE with respect to each w_j and setting them to zero

$$\begin{aligned} \frac{\partial}{\partial w_j} SSE &= \sum_{i=1}^t 2(\mathbf{w} \cdot \mathbf{x}_i - y_i) x_{ij} \\ &= 2\left(\sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{ij} - \sum_{i=1}^t y_i x_{ij} \right) \end{aligned}$$

Thus, consider whole vector of derivatives

$$
\begin{aligned}
\nabla_{\mathbf{w}} SSE &= \begin{bmatrix} \frac{\partial SSE}{\partial w_1} \\ \frac{\partial SSE}{\partial w_2} \\ \vdots \\ \frac{\partial SSE}{\partial w_n} \end{bmatrix} = \begin{bmatrix} 2\left(\sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{i1} - \sum_{i=1}^t y_i x_{i1}\right) \\ 2\left(\sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{i2} - \sum_{i=1}^t y_i x_{i2}\right) \\ \vdots \\ 2\left(\sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{in} - \sum_{i=1}^t y_i x_{in}\right) \end{bmatrix} \\
&= 2 \begin{bmatrix} \sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{i1} \\ \sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{i2} \\ \vdots \\ \sum_{i=1}^t \sum_{k=1}^n w_k x_{ik} x_{in} \end{bmatrix} - 2 \begin{bmatrix} \sum_{i=1}^t y_i x_{i1} \\ \sum_{i=1}^t y_i x_{i2} \\ \vdots \\ \sum_{i=1}^t y_i x_{in} \end{bmatrix} \\
&= 2X^T \begin{bmatrix} \sum_{k=1}^n w_k x_{1k} \\ \sum_{k=1}^n w_k x_{2k} \\ \vdots \\ \sum_{k=1}^n w_k x_{tk} \end{bmatrix} - 2X^T \mathbf{y} \\
&= 2X^T X \mathbf{w} - 2X^T \mathbf{y}
\end{aligned}
$$

Now solve for $\mathbf{w}$ that makes this vector of derivatives equal to zero

$$
\begin{aligned}
2X^T X \mathbf{w} - 2X^T \mathbf{y} &= 0 \\
X^T X \mathbf{w} &= X^T \mathbf{y} \\
\mathbf{w} &= (X^T X)^{-1} X^T \mathbf{y}
\end{aligned}
$$

Or in Matlab

$$
\mathbf{w} = (X^T X) \setminus (X^T \mathbf{y})
$$

This $\mathbf{w}$ is unique if the columns of X are independent

22.2 Geometric derivation

Think of columns of X as vectors

$$\begin{bmatrix} \begin{bmatrix} \mathbf{v}_1 \end{bmatrix} & \begin{bmatrix} \mathbf{v}_2 \end{bmatrix} & \cdots & \begin{bmatrix} \mathbf{v}_n \end{bmatrix} \end{bmatrix}$$

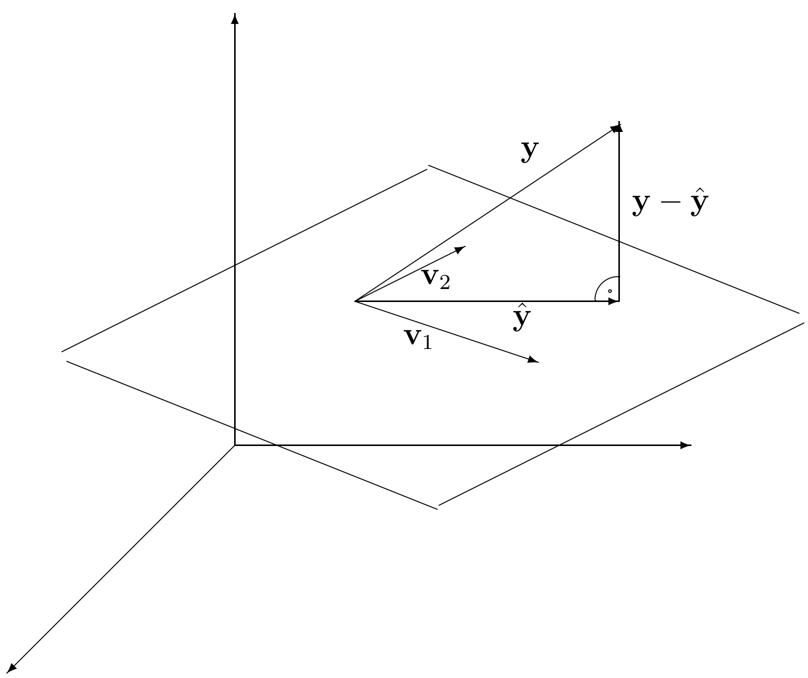
Looking for linear combination of columns that best approximates $\mathbf{y}$

For any weight vector $\mathbf{w}$ get

$$\hat{y} = w_1\mathbf{v}_1 + w_2\mathbf{v}_2 + \ldots + w_n\mathbf{v}_n$$

Any such $\hat{y}$ lies in span$(\mathbf{v}_1, \ldots, \mathbf{v}_n)$

The element $\hat{\mathbf{y}}$ of span$(\mathbf{v}_1, \ldots, \mathbf{v}_n)$ that minimizes $||\hat{\mathbf{y}} - \mathbf{y}||^2$ is given by the orthogonal projection of $\mathbf{y}$ onto span$(\mathbf{v}_1, \ldots, \mathbf{v}_n)$



Since the vector $\mathbf{y} - \hat{\mathbf{y}}$ is orthogonal to span$(\mathbf{v}_1, \ldots, \mathbf{v}_n)$, the inner products $\mathbf{v}_i(\mathbf{y} - \hat{\mathbf{y}})$ are zero. That is, $\mathbf{v}_i \cdot \hat{\mathbf{y}} = \mathbf{v}_i \cdot \mathbf{y}$ for all $i = 1 \ldots n$

The vectors $\mathbf{v}_i$ are columns of the matrix X, so the equalities can be rewritten

$$X^T\hat{\mathbf{y}} \;=\; X^T\mathbf{y}$$

Remembering that $\hat{\mathbf{y}} = X\mathbf{w}$, we finally get

$$X^T X\mathbf{w} \;=\; X^T\mathbf{y}$$

Same as before

22.3 Other error functions

Sum of squared errors is not always the best error function

For example, could use

$$\begin{aligned} \mathrm{err}(\hat{\mathbf{y}},\mathbf{y}) \;=\; & \textstyle\sum_i(\hat{y}_i - y_i)^2 && L_2 \text{ error} \\ & \textstyle\sum_i|\hat{y}_i - y_i| && L_1 \text{ error} \\ & \textstyle\sum_i|\hat{y}_i - y_i|^p && L_p \text{ error} \\ & \max_i|\hat{y}_i - y_i| && L_\infty \text{ error} \end{aligned}$$

Example: Minimize maximum training error (L_∞)

- Choose $\mathbf{w}$ to minimize $\max_i|\mathbf{w}\cdot\mathbf{x}_i - y_i|$
- Linear programming: find $\mathbf{w},\delta$ to minimize δ, subject to constraints

$$\begin{aligned} \mathbf{w}\cdot\mathbf{x}_1 &\leq y_1 + \delta \\ \mathbf{w}\cdot\mathbf{x}_1 &\geq y_1 - \delta \\ \vdots \;&\;\vdots\;\;\vdots \\ \mathbf{w}\cdot\mathbf{x}_t &\leq y_t + \delta \\ \mathbf{w}\cdot\mathbf{x}_t &\geq y_t - \delta \end{aligned}$$

- Can be done in polynomial time

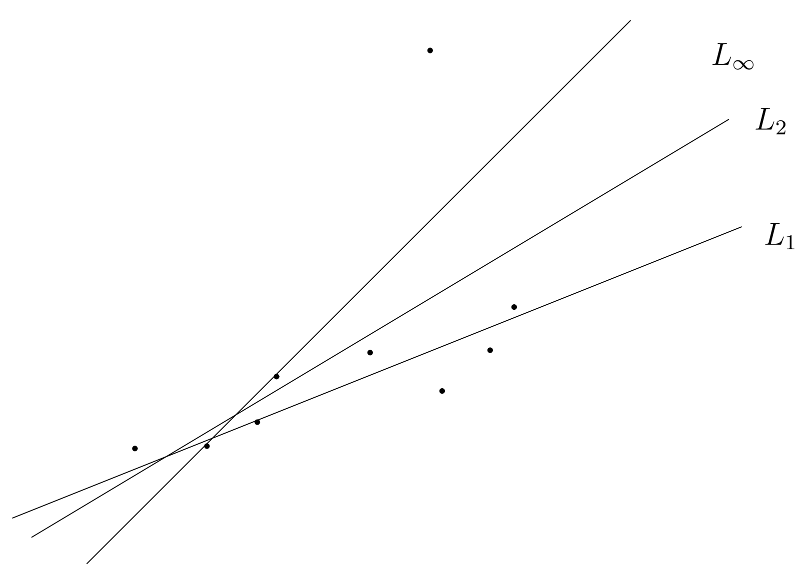
Example: Minimize sum of absolute error (L_1)

- Choose w to minimize $\sum_{i=1}^{t} |\mathbf{w} \cdot \mathbf{x}_i - y_i|$
- Linear programming: choose $\mathbf{w}, \boldsymbol{\delta}$ to minimize $\sum_{i=1}^{t} |\delta_i| = \sum_{i=1}^{t} \delta_i^+ + \delta_i^-$ subject to

$$
\begin{array}{rclcl}
\mathbf{w} \cdot \mathbf{x}_1 + \delta_1 & = & \mathbf{w} \cdot \mathbf{x}_1 + \delta_1^+ - \delta_1^- & = & y_1 \\
\mathbf{w} \cdot \mathbf{x}_2 + \delta_2 & = & \mathbf{w} \cdot \mathbf{x}_2 + \delta_2^+ - \delta_2^- & = & y_2 \\
\vdots & & \vdots & & \\
\mathbf{w} \cdot \mathbf{x}_t + \delta_t & = & \mathbf{w} \cdot \mathbf{x}_t + \delta_t^+ - \delta_t^- & = & y_t
\end{array}
$$

Which objective is best?

- L_1 is the most robust against outliers
- L_2 is cheapest computationally
- L_∞ gives the best upper bound on training set error

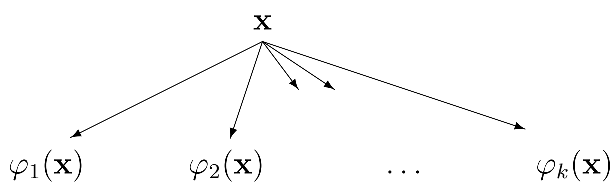


22.4 Generalized linear functions

Linear functions may not be expressive enough

Trick expand representation $\mathbf{x} \mapsto \boldsymbol{\varphi}(\mathbf{x})$

Define new attributes which are non-linear functions of original attributes



"basis functions"

Expand training set

$$\left[\begin{array}{ccc|c} x_{11} & \dots & x_{1n} & y_1 \\ x_{21} & \dots & x_{2n} & y_2 \\ \vdots & \ddots & \vdots & \vdots \\ x_{t1} & \dots & x_{tn} & y_t \end{array}\right]$$

$$\Downarrow$$

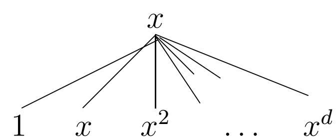
$$\underbrace{\left[\begin{array}{ccc|c} \varphi_1(\mathbf{x}_1) & \dots & \varphi_k(\mathbf{x}_1) & y_1 \\ \varphi_1(\mathbf{x}_2) & \dots & \varphi_k(\mathbf{x}_2) & y_2 \\ \vdots & \ddots & \vdots & \vdots \\ \varphi_1(\mathbf{x}_t) & \dots & \varphi_k(\mathbf{x}_t) & y_t \end{array}\right]}_{\Phi \qquad\qquad \mathbf{y}}$$

Learn a linear function over expanded representation, which is *non-linear* in the original representation

E.g. learn non-linear function to minimize L_2 error by solving for $\mathbf{w}$ such that $\Phi^T\Phi\mathbf{w} = \Phi^T\mathbf{y}$

Example: Polynomial regression

Let $X = \Re$, and use the expanded set of all powers of x, up to d



Expand training set

$$\begin{matrix} (x_1, y_1) \\ (x_2, y_2) \\ \vdots \\ (x_t, y_t) \end{matrix} \quad \Rightarrow \quad \left[\begin{array}{ccccc|c} 1 & x_1 & x_1^2 & \ldots & x_1^d & y_1 \\ 1 & x_2 & x_2^2 & \ldots & x_2^d & y_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & x_t & x_t^2 & \ldots & x_t^d & y_t \end{array} \right]$$

To find the best polynomial, solve for $\mathbf{w}$ in $\Phi^T \Phi \mathbf{w} = \Phi^T \mathbf{y}$
Obtain coefficients of minimal squared error polynomial of degree d

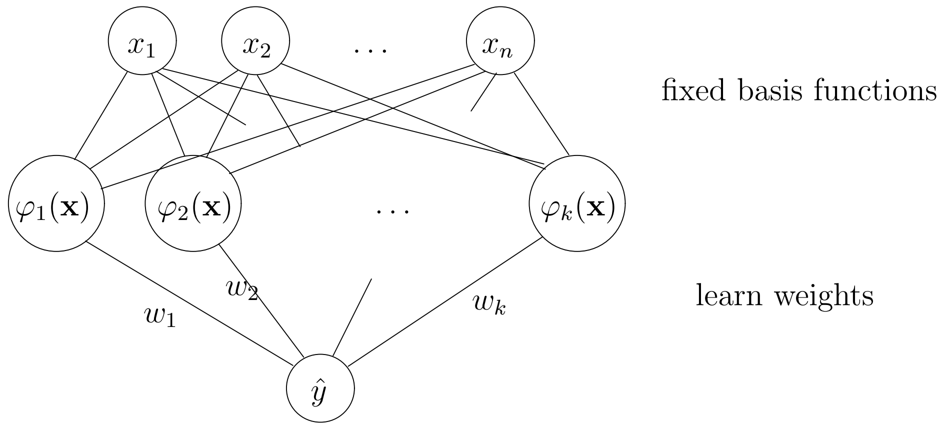
(Can also easily solve for min abosolute error, and min maximum error polynomials, by exploiting the same basis expansion and using the linear programming formulations shown earlier to calculate $\mathbf{w}$)

Other basis functions

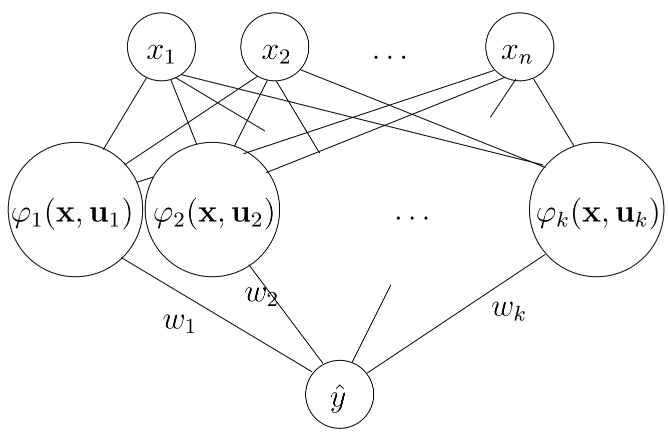
- spline fitting (basis splines)
- radial basis functions
- Fourier analysis

22.5 Neural networks

Learning a generalized linear function could be depicted as



However, in addition to the weights $\mathbf{w}$ at the final level, we could also try to learn the basis functions φ_i themselves. So add parameters $\mathbf{u}_i$ to φ_i, and attempt to learn $\mathbf{u}_i$ parameters in addition to $\mathbf{w}$ parameters



In total, have to learn weights $\mathbf{w}$, $U = [\mathbf{u}_1; \ldots; \mathbf{u}_k]$ to minimize *SSE*

- Unfortunately, the problem is *NP-hard*. There is no general polynomial time training procedure.

- Can use gradient descent optimization in $\mathbf{w}, U$ to heuristically find a local minimum

"Backpropagation algorithm"

- Uses efficient scheme for calculating weight gradients using chain rule of differentiation

Readings

Russell and Norvig 2nd Ed: Chapter 20
Dean, Allen, Aloimonos: Sections 5.5, 5.6, 5.8
Hastie, Tibshirani, Friedman: Chapters 2, 3, 11