Machine learning: lecture 6

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Topics

- Generalized linear models (cont'd)
  - logistic regression
  - gradient ascent, learning rate, convergence, examples
  - additive models, neural networks, back-propagation
- Regularization
  - basic idea
  - effective number of parameters

Review: logistic regression

- In a logistic regression model the conditional probability of the label y given the input example $\mathbf{x}$ is expressed as

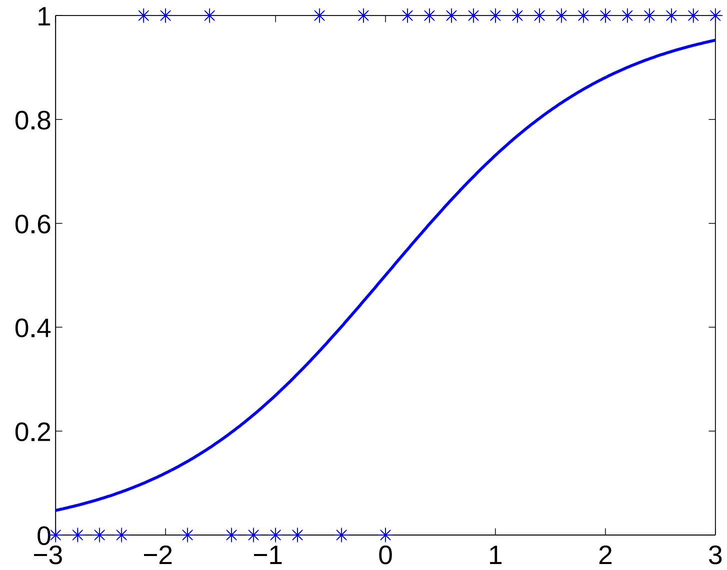
$$P(y = 1|\mathbf{x}, \mathbf{w}) = g\left(w_0 + w_1 x_1 + \ldots + w_d x_d \right)$$

where the coefficients $\mathbf{w}$ are the adjustable parameters.

The "squashing function"

$$g(z) = (1 + \exp(-z))^{-1}$$

known as the logistic function turns linear predictions into probabilities



Example problem

- The problem: classification of radar returns from the ionosphere (data is available from the UCI ML repository)
  - binary class label
  - 34 input "features" (2 values per radar pulse) defining the input vector $\mathbf{x} = [x_1, \ldots, x_{34}]^T$.
  - 200 training and 150 testing examples

- We would like to estimate a simple logistic regression model for this classification task

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g\left(w_0 + w_1 x_1 + \ldots + w_d x_d \right)$$

where $d = 34$.

Fitting logistic regression models

- As in the case of linear regression models we can fit the logistic models using the maximum log-likelihood criterion

$$l(D; \mathbf{w}) = \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i, \mathbf{w})$$

where

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g\left(w_0 + w_1 x_1 + \ldots + w_d x_d \right)$$

- The log-likelihood function $l(D; \mathbf{w})$ is a *concave* function of the parameters $\mathbf{w}$; a number of optimization techniques are available for finding the maximizing parameters

Gradient ascent

- We can maximize the log-likelihood by iteratively adjusting the parameters in small increments

  In each iteration we adjust $\mathbf{w}$ slightly in the direction that increases the log-likelihood (towards the gradient):

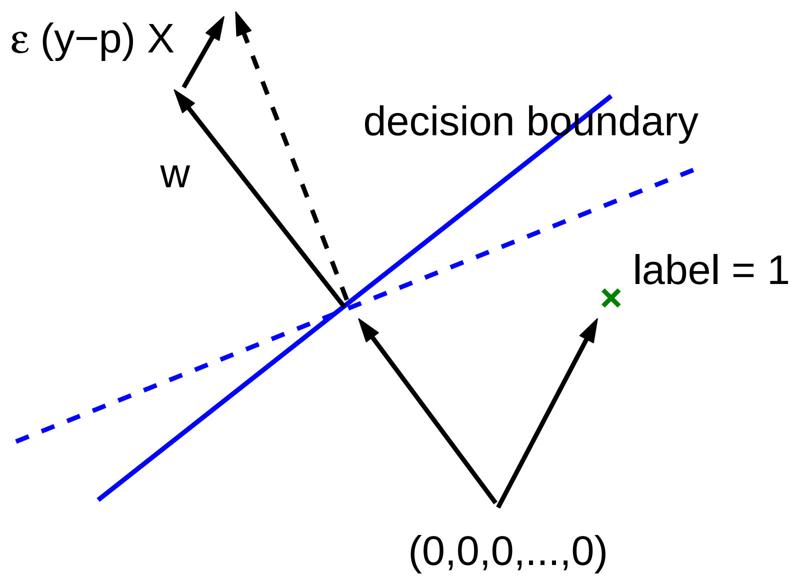
$$
\begin{aligned}
\mathbf{w} &\leftarrow \mathbf{w} + \epsilon \frac{\partial}{\partial \mathbf{w}} \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i, \mathbf{w}) \\
&= \cdots \\
&= \mathbf{w} + \epsilon \sum_{i=1}^{n} \underbrace{\Big(y_i - P(y_i = 1|\mathbf{x}_i, \mathbf{w}) \Big)}_{\text{prediction error}} \begin{bmatrix} 1 \\ \mathbf{x}_i \end{bmatrix}
\end{aligned}
$$

where ϵ is the *learning rate*.

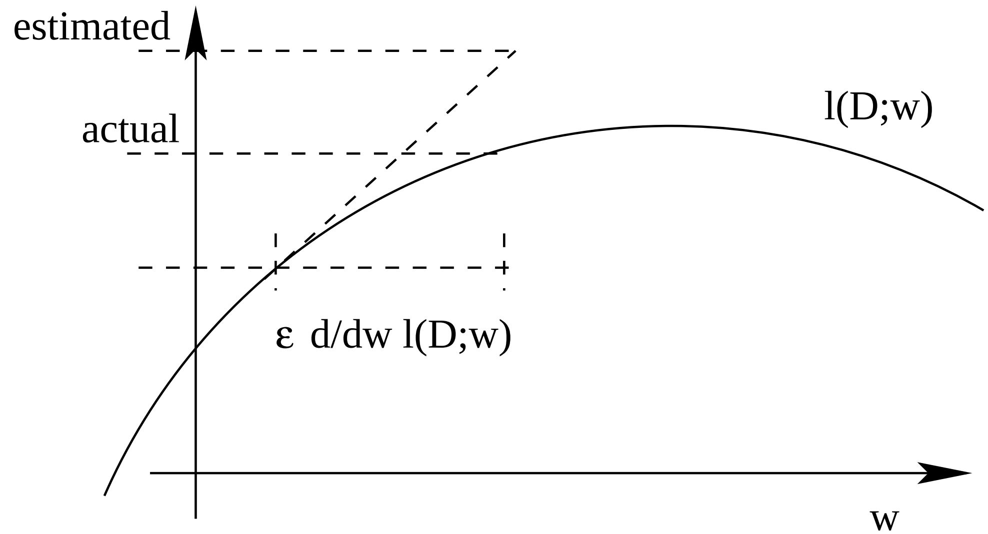
Gradient ascent cont'd

- To understand the procedure graphically we can focus on a single example

$$\mathbf{w} \;\leftarrow\; \mathbf{w} + \epsilon \underbrace{\left(y_i - P(y_i = 1 | \mathbf{x}_i, \mathbf{w}) \right)}_{\text{prediction error}} \begin{bmatrix} 1 \\ \mathbf{x}_i \end{bmatrix}$$



Setting the learning rate: Armijo rule



The learning rate in

$$\mathbf{w} \leftarrow \mathbf{w} + \epsilon \frac{\partial}{\partial \mathbf{w}} l(D; \mathbf{w})$$

"should" satisfy

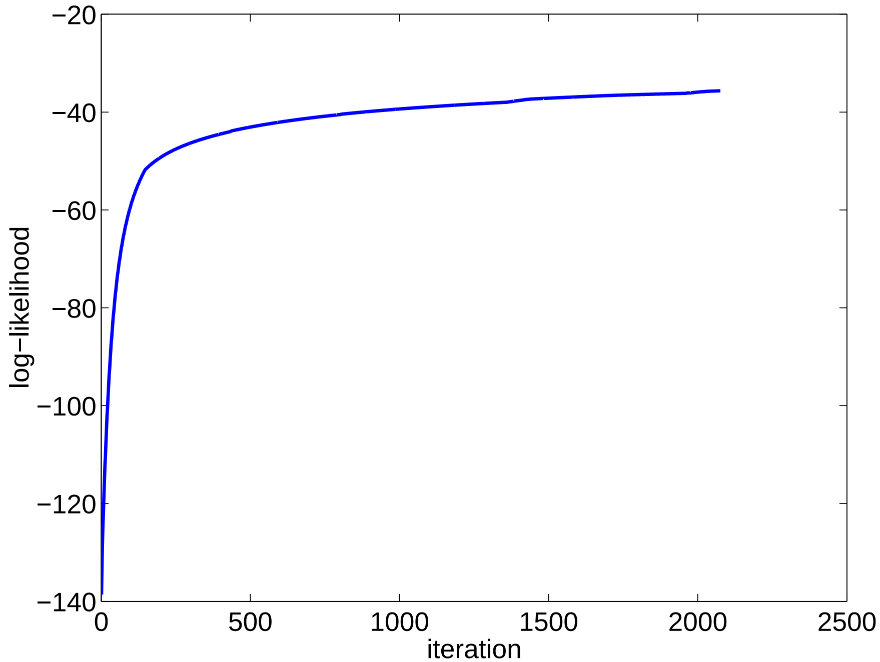
$$l\left(D;\, \mathbf{w} + \epsilon \frac{\partial}{\partial \mathbf{w}} l(D; \mathbf{w})\right) - l(D; \mathbf{w}) \geq \epsilon \cdot \frac{1}{2} \| \frac{\partial}{\partial \mathbf{w}} l(D; \mathbf{w}) \|^2$$

The Armijo rule suggests finding the smallest integer m such that $\epsilon = \epsilon_0 q^m,\ q < 1$ is a valid choice in this sense.

- Armijo rule is guaranteed to converge to a (local) maximum under certain technical assumptions

Example cont'd

- We get a monotonically increasing log-likelihood of the training labels as a function of the gradient ascent iterations



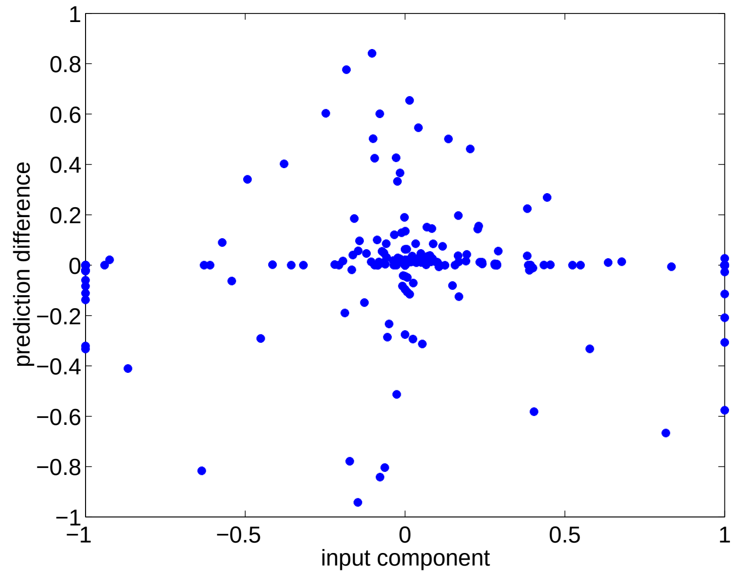
- The resulting error rate on the (independent) test set is %9.3

Gradient ascent: convergence

- The gradient ascent learning method *converges* when there is no incentive to move the parameters in any particular direction:

$$\sum_{i=1}^{n} \underbrace{\left(y_i - P(y_i = 1 | \mathbf{x}_i, \hat{\mathbf{w}}) \right)}_{\text{prediction error}} \begin{bmatrix} 1 \\ \mathbf{x}_i \end{bmatrix} = 0$$

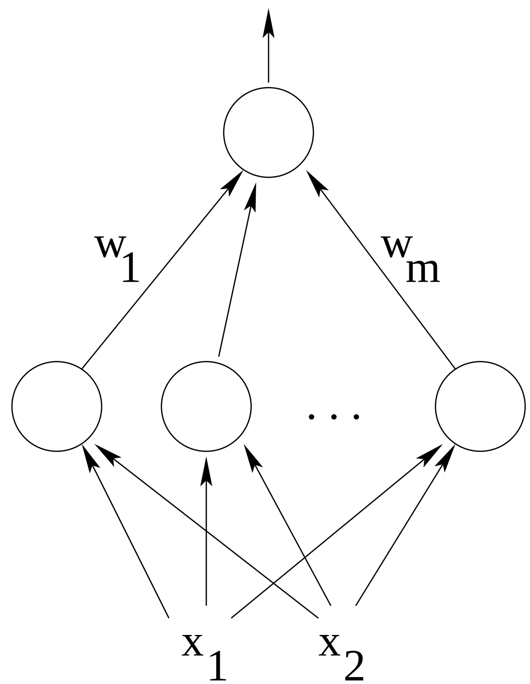
- This condition means again that the prediction error is decorrelated with the components of the input vector



Additive models and classification

- Similarly to linear regression models, we can extend the logistic regression models to additive (logistic) models

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g\,(\,w_0 + w_1\phi_1(\mathbf{x}) + \ldots w_m\phi_m(\mathbf{x})\,)$$

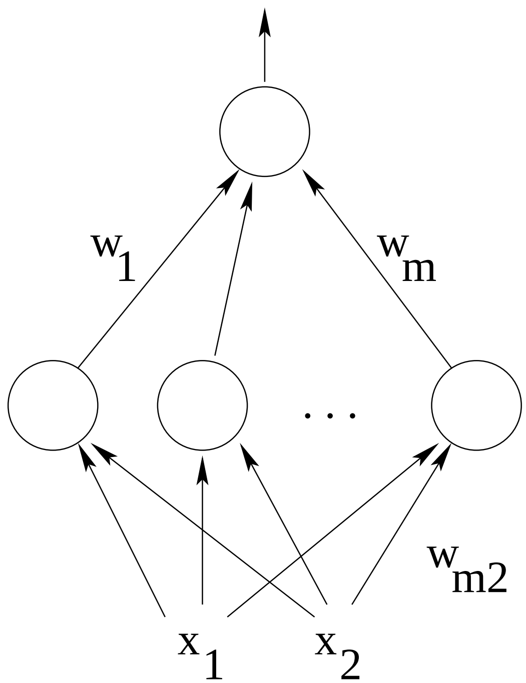


- We are again free to choose the basis functions $\phi_i(\mathbf{x})$

Two layer neural network model

- In a neural network model, the basis functions themselves are adjustable (e.g., squashed linear regression models) representing the probability that a "feature" is present in the input

$$P(y=1|\mathbf{x},\mathbf{w}) \;=\; g\,(\,w_0 + w_1\phi_1(\mathbf{x}) + \ldots w_m\phi_m(\mathbf{x})\,)$$

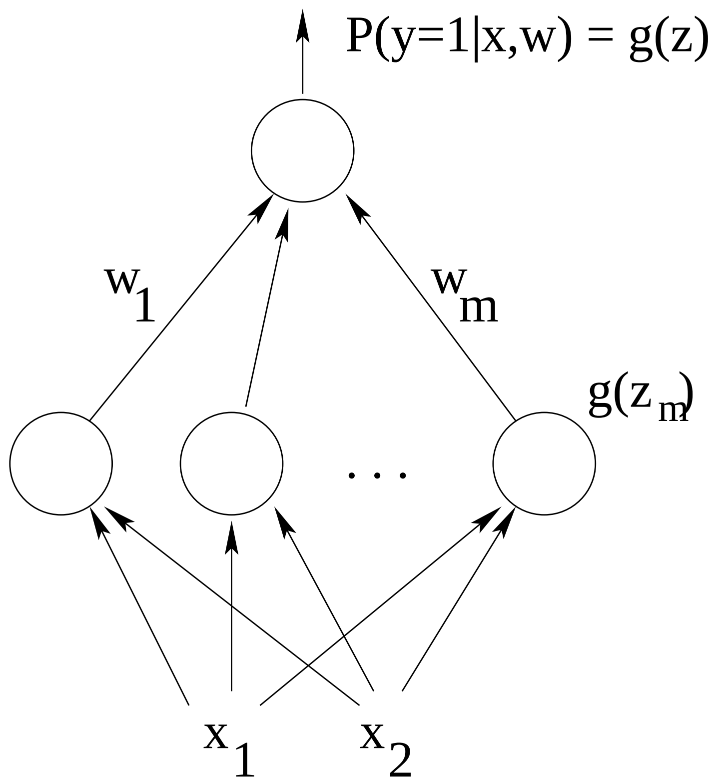


$$\phi_m(x) = g(\,w_{m0} + w_{m1}x_1 + w_{m2}x_2\,)$$

Computing the gradient: back-propagation

Let z, $z_i, i = 1, \ldots, m$ be the total "input" to each "node" computed in response to a training example $\mathbf{x}$

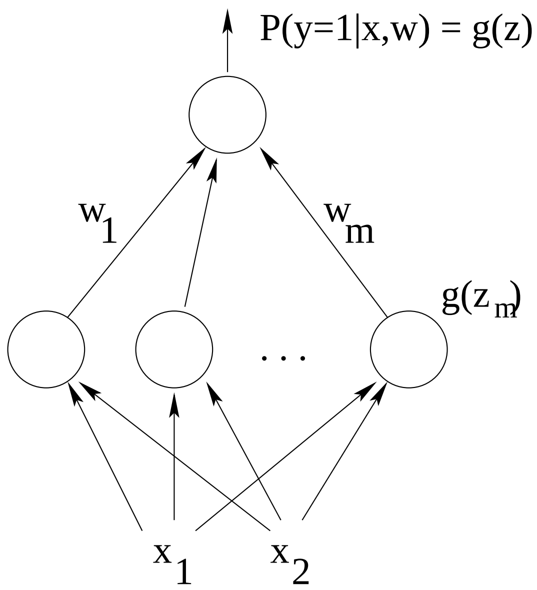
$$
\begin{aligned}
z &= w_0 + w_1 g(z_1) + \ldots + w_m g(z_m) \\
z_i &= w_{i0} + w_{i1} x_1 + w_{i2} x_2, \;\; i = 1, \ldots, m
\end{aligned}
$$



Back-propagation cont'd

- We can propagate the derivatives with respect to the *inputs*

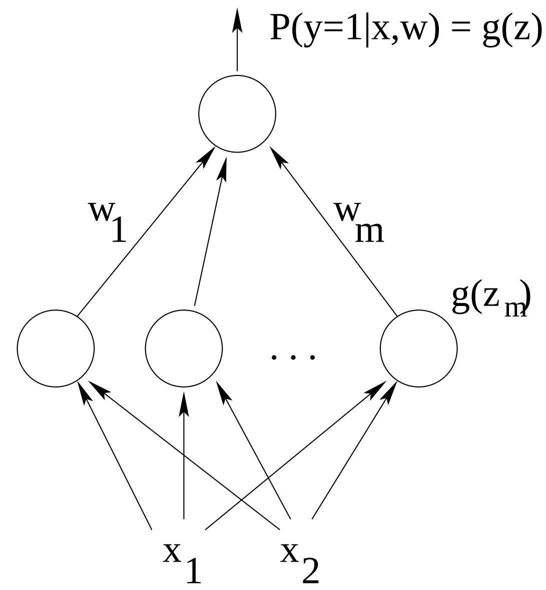
$$\begin{aligned}
\delta &= \frac{\partial}{\partial z} \log P(y|\mathbf{x}, \mathbf{w}) \\
\delta_i &= \frac{\partial}{\partial z_i} \log P(y|\mathbf{x}, \mathbf{w}) \\
&= \frac{\partial g(z_i)}{\partial z_i} \times \frac{\partial z}{\partial g(z_i)} \times \frac{\partial}{\partial z} \log P(y|\mathbf{x}, \mathbf{w}) \\
&= g'(z_i) \times w_i \times \delta
\end{aligned}$$



Back-propagation cont'd

- We can propagate the derivatives with respect to the *inputs*

$$\begin{aligned} \delta &= \frac{\partial}{\partial z} \log P(y|\mathbf{x}, \mathbf{w}) \\ \delta_i &= \frac{\partial}{\partial z_i} \log P(y|\mathbf{x}, \mathbf{w}) \\ &= \frac{\partial g(z_i)}{\partial z_i} \times \frac{\partial z}{\partial g(z_i)} \times \frac{\partial}{\partial z} \log P(y|\mathbf{x}, \mathbf{w}) \\ &= g'(z_i) \times w_i \times \delta \end{aligned}$$



- The derivatives with respect to the weights w_{ij} are obtained from δ's

$$\frac{\partial}{\partial w_{ij}} \log P(y|\mathbf{x}, \mathbf{w}) = \frac{\partial z_i}{\partial w_{ij}} \times \frac{\partial}{\partial z_i} \log P(y|\mathbf{x}, \mathbf{w}) = x_j \times \delta_i$$

Topics

- Regularization
  - basic idea
  - effective number of parameters

The key idea ... is to limit "choices"

Questions to answer:

1. What are the "choices"?
2. How do we limit the choices?
3. Why do we need to limit the choices? (next lecture)

Example

- The set of (0/1) coins parameterized by the probability p of getting "1"

  How many coins are there?

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  Case 1: ∞
  Case 2: 9 coins $(p_1, \ldots, p_9)$ so that predictions of any other coin (indexed by p) is no more than $\epsilon = 0.1$ away

  for any p, $|p - p_j| \leq \epsilon$ for at least one j

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  for any p, $|p - p_j| \leq \epsilon$ for at least one j

  Case 3: only 1 coin if $\epsilon = 0.5$

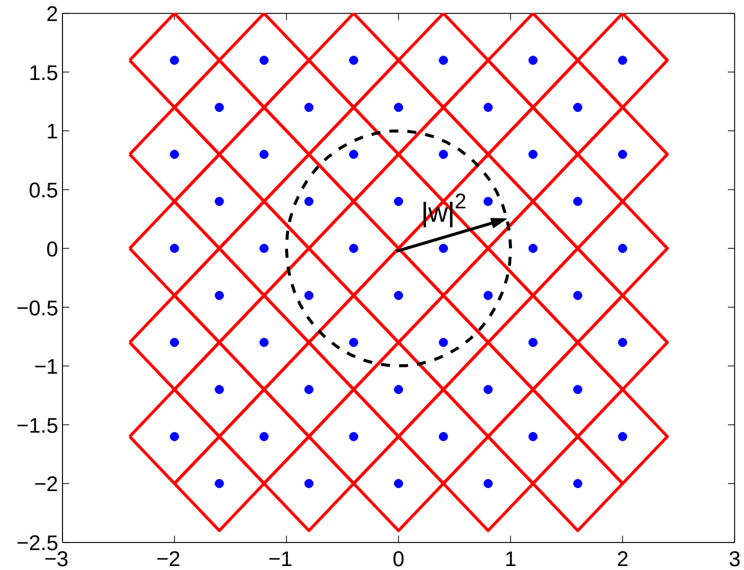
Logistic regression example

- Simple logistic regression model

$$P(y = 1|x, \mathbf{w}) = g(w_0 + w_1 x)$$

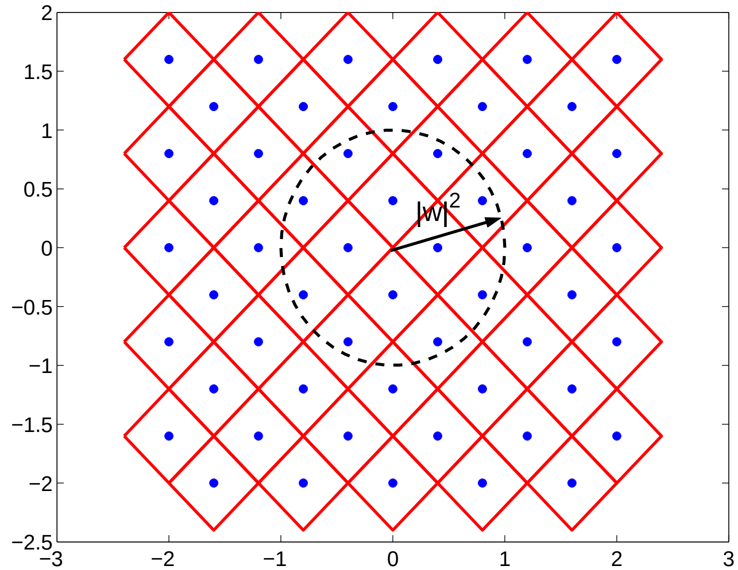
parameterized by $\mathbf{w} = (w_0, w_1)$. We assume that $x \in [-1, 1]$, i.e., that the inputs remain bounded.

- We can now divide the parameter space into regions with centers $\mathbf{w}_1, \mathbf{w}_2, \ldots$ such that the predictions of any $\mathbf{w}$ (for any $x \in [-1, 1]$) are close to those of one of the centers:



$$|\log P(y = 1|x, \mathbf{w}) - \log P(y = 1|x, \mathbf{w}_j)| \leq \epsilon$$

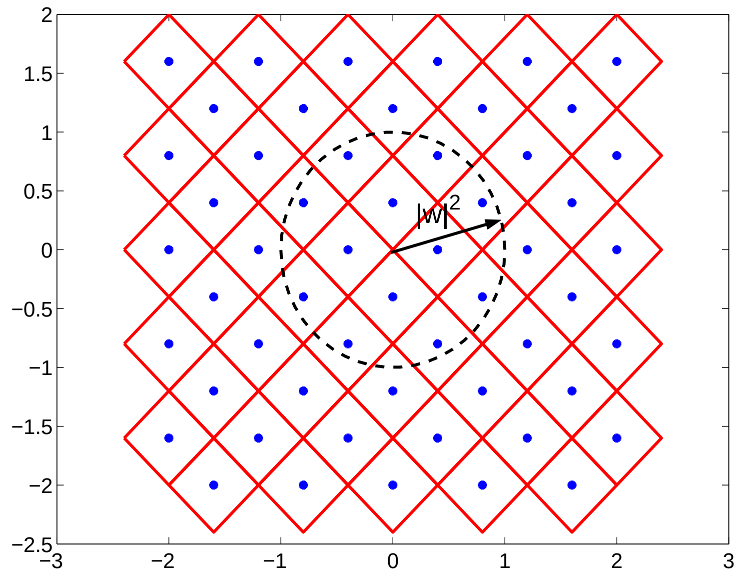
Limiting choices: regularization



- By constraining $\|\mathbf{w}\| \leq C$ for some *regularization parameter* C, we have fewer effective parameter choices in the logistic regression model

$$P(y = 1|x, \mathbf{w}) = g(w_0 + w_1 x)$$

Regularization cont'd



- We can also regularize by imposing a penalty in the estimation criterion that encourages $\|\mathbf{w}\|$ to remain small.

  Maximum penalized likelihood

$$l(D; \mathbf{w}, \lambda) = \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i, \mathbf{w}) - \frac{\lambda}{2}\|\mathbf{w}\|^2$$

  where larger values of λ impose stronger regularization.