CSC 2515 Lecture 4: Linear Models II

Marzyeh Ghassemi

Material and slides developed by Roger Grosse, University of Toronto

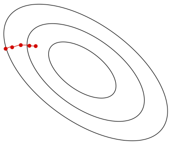
Today's Agenda

Today's agenda:

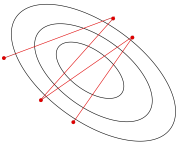
- **Optimization**
  - **choice of learning rate**
  - **stochastic gradient descent**
- Multiclass classification
  - softmax regression
- L^1 regularization
- Support vector machines
- Boosting

Learning Rate

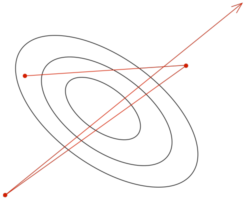
- In gradient descent, the learning rate α is a hyperparameter we need to tune. Here are some things that can go wrong:



α too small: slow progress



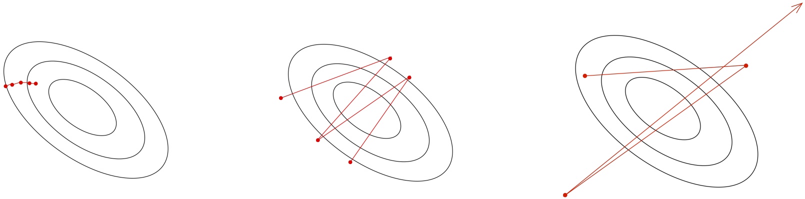
α too large: oscillations



α much too large: instability

Learning Rate

- In gradient descent, the learning rate α is a hyperparameter we need to tune. Here are some things that can go wrong:



α too small: slow progress

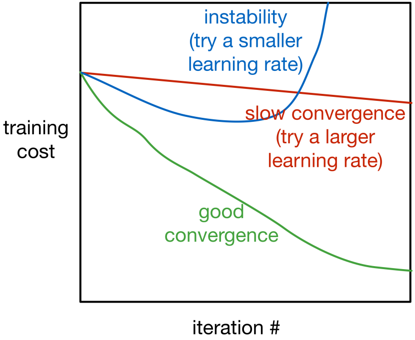
α too large: oscillations

α much too large: instability

- Good values are typically between 0.001 and 0.1. You should do a grid search if you want good performance (i.e. try $0.1, 0.03, 0.01, \ldots$).

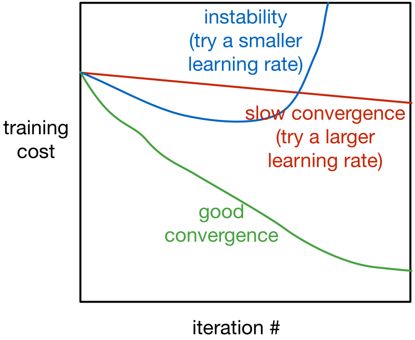
Training Curves

- To diagnose optimization problems, it's useful to look at training curves: plot the training cost as a function of iteration.



Training Curves

- To diagnose optimization problems, it's useful to look at training curves: plot the training cost as a function of iteration.



- Warning: it's very hard to tell from the training curves whether an optimizer has converged. They can reveal major problems, but they can't guarantee convergence.

Stochastic Gradient Descent

- So far, the cost function $\mathcal{J}$ has been the average loss over the training examples:

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}^{(i)} = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(y(\mathbf{x}^{(i)}, \boldsymbol{\theta}), t^{(i)}).$$

- By linearity,

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}} = \frac{1}{N}\sum_{i=1}^{N}\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}.$$

Stochastic Gradient Descent

- So far, the cost function $\mathcal{J}$ has been the average loss over the training examples:

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}^{(i)} = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(y(\mathbf{x}^{(i)},\boldsymbol{\theta}), t^{(i)}).$$

- By linearity,

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}} = \frac{1}{N}\sum_{i=1}^{N}\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}.$$

- Computing the gradient requires summing over *all* of the training examples. This is known as batch training.
- Batch training is impractical if you have a large dataset (e.g. millions of training examples)!

Stochastic Gradient Descent

- Stochastic gradient descent (SGD): update the parameters based on the gradient for a single training example:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}$$

- SGD can make significant progress before it has even looked at all the data!

Stochastic Gradient Descent

- Stochastic gradient descent (SGD): update the parameters based on the gradient for a single training example:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}$$

- SGD can make significant progress before it has even looked at all the data!
- Mathematical justification: if you sample a training example at random, the stochastic gradient is an unbiased estimate of the batch gradient:

$$\mathbb{E}\left[\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}\right] = \frac{1}{N}\sum_{i=1}^{N}\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}.$$

- Problem:

Stochastic Gradient Descent

- Stochastic gradient descent (SGD): update the parameters based on the gradient for a single training example:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}$$

- SGD can make significant progress before it has even looked at all the data!
- Mathematical justification: if you sample a training example at random, the stochastic gradient is an unbiased estimate of the batch gradient:

$$\mathbb{E}\left[\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}\right] = \frac{1}{N}\sum_{i=1}^{N} \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}.$$

- Problem: if we only look at one training example at a time, we can't exploit efficient vectorized operations.

Stochastic Gradient Descent

- Compromise approach: compute the gradients on a medium-sized set of training examples, called a mini-batch.
  - Conceptually, it's useful to think of mini-batches as sampled i.i..d. from the training set.
  - In practice, we typically go in order through the training set.
  - Each entire pass over the dataset is called an epoch.

Stochastic Gradient Descent

- Compromise approach: compute the gradients on a medium-sized set of training examples, called a mini-batch.
  - Conceptually, it's useful to think of mini-batches as sampled i.i..d. from the training set.
  - In practice, we typically go in order through the training set.
  - Each entire pass over the dataset is called an epoch.
- If mini-batches are independent, the stochastic gradients computed on larger mini-batches have smaller variance:

$$\mathrm{Var}\left[\frac{1}{S}\sum_{i=1}^{S}\frac{\partial \mathcal{L}^{(i)}}{\partial \theta_j}\right] = \frac{1}{S^2}\,\mathrm{Var}\left[\sum_{i=1}^{S}\frac{\partial \mathcal{L}^{(i)}}{\partial \theta_j}\right] = \frac{1}{S}\,\mathrm{Var}\left[\frac{\partial \mathcal{L}^{(i)}}{\partial \theta_j}\right]$$

Stochastic Gradient Descent

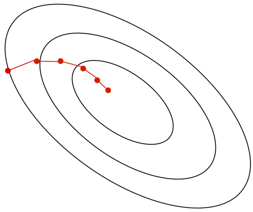
- Compromise approach: compute the gradients on a medium-sized set of training examples, called a mini-batch.
  - Conceptually, it's useful to think of mini-batches as sampled i.i..d. from the training set.
  - In practice, we typically go in order through the training set.
  - Each entire pass over the dataset is called an epoch.
- If mini-batches are independent, the stochastic gradients computed on larger mini-batches have smaller variance:

$$\mathrm{Var}\left[\frac{1}{S}\sum_{i=1}^{S}\frac{\partial\mathcal{L}^{(i)}}{\partial\theta_j}\right] = \frac{1}{S^2}\,\mathrm{Var}\left[\sum_{i=1}^{S}\frac{\partial\mathcal{L}^{(i)}}{\partial\theta_j}\right] = \frac{1}{S}\,\mathrm{Var}\left[\frac{\partial\mathcal{L}^{(i)}}{\partial\theta_j}\right]$$

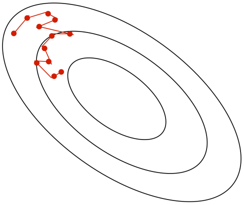
- The mini-batch size S is a hyperparameter that needs to be set.
  - Too large: takes more memory to store the activations, and longer to compute each gradient update
  - Too small: can't exploit vectorization
  - A reasonable value might be $S = 100$.

Stochastic Gradient Descent

- Batch gradient descent moves directly downhill. SGD takes steps in a noisy direction, but moves downhill on average.



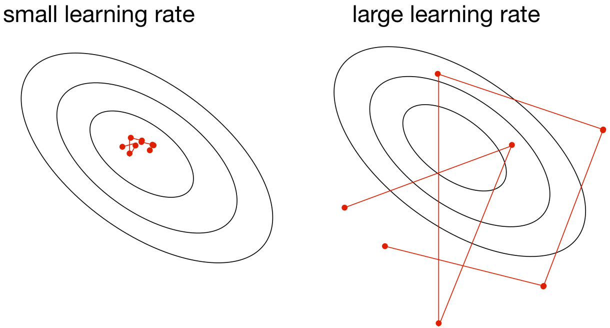
batch gradient descent



stochastic gradient descent

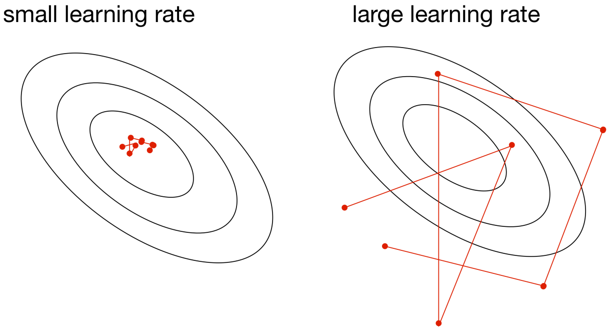
SGD Learning Rate

- In stochastic training, the learning rate also influences the fluctuations due to the stochasticity of the gradients.



SGD Learning Rate

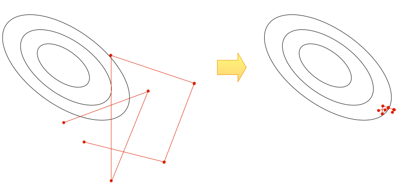
- In stochastic training, the learning rate also influences the fluctuations due to the stochasticity of the gradients.

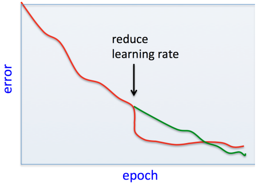


- Typical strategy:
  - Use a large learning rate early in training so you can get close to the optimum
  - Gradually decay the learning rate to reduce the fluctuations

SGD Learning Rate

- Warning: by reducing the learning rate, you reduce the fluctuations, which can appear to make the loss drop suddenly. But this can come at the expense of long-run performance.





Questions?

?

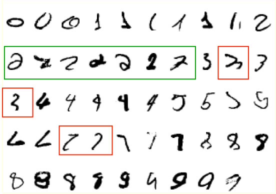
Today's Agenda

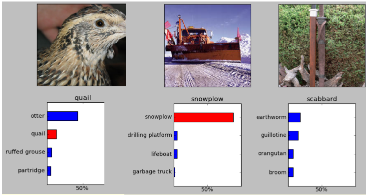
Today's agenda:

- Optimization
  - choice of learning rate
  - stochastic gradient descent
- **Multiclass classification**
  - **softmax regression**
- L^1 regularization
- Support vector machines
- Boosting

Multiclass Classification

- What about classification tasks with more than two categories?





Multiclass Classification

- Targets form a discrete set $\{1, \ldots, K\}$.
- It's often more convenient to represent them as one-hot vectors, or a one-of-K encoding:

$$\mathbf{t} = \underbrace{(0, \ldots, 0, 1, 0, \ldots, 0)}_{\text{entry } k \text{ is } 1}$$

Multiclass Classification

- Now there are D input dimensions and K output dimensions, so we need $K \times D$ weights, which we arrange as a weight matrix $\mathbf{W}$.
- Also, we have a K-dimensional vector $\mathbf{b}$ of biases.
- Linear predictions:

$$z_k = \sum_j w_{kj} x_j + b_k$$

- Vectorized:

$$\mathbf{z} = \mathbf{W}\mathbf{x} + \mathbf{b}$$

Multiclass Classification

- A natural activation function to use is the softmax function, a multivariable generalization of the logistic function:

$$y_k = \mathrm{softmax}(z_1, \ldots, z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

- The inputs z_k are called the logits.

Multiclass Classification

- A natural activation function to use is the softmax function, a multivariable generalization of the logistic function:

$$y_k = \mathrm{softmax}(z_1, \ldots, z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

- The inputs z_k are called the logits.
- Properties:
  - Outputs are positive and sum to 1 (so they can be interpreted as probabilities)
  - If one of the z_k's is much larger than the others, $\mathrm{softmax}(\mathbf{z})$ is approximately the argmax. (So really it's more like "soft-argmax".)

Multiclass Classification

- A natural activation function to use is the softmax function, a multivariable generalization of the logistic function:

$$y_k = \mathrm{softmax}(z_1, \ldots, z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

- The inputs z_k are called the logits.
- Properties:
  - Outputs are positive and sum to 1 (so they can be interpreted as probabilities)
  - If one of the z_k's is much larger than the others, $\mathrm{softmax}(\mathbf{z})$ is approximately the argmax. (So really it's more like "soft-argmax".)
- Note: sometimes $\sigma(\mathbf{z})$ is used to denote the softmax function; in this class, it will denote the logistic function applied elementwise.

Multiclass Classification

- If a model outputs a vector of class probabilities, we can use cross-entropy as the loss function:

$$
\begin{aligned}
\mathcal{L}_{\mathrm{CE}}(\mathbf{y}, \mathbf{t}) &= -\sum_{k=1}^{K} t_k \log y_k \\
&= -\mathbf{t}^\top (\log \mathbf{y}),
\end{aligned}
$$

  where the log is applied elementwise.

- Just like with logistic regression, we typically combine the softmax and cross-entropy into a softmax-cross-entropy function.

Multiclass Classification

- Softmax regression:

$$
\begin{aligned}
\mathbf{z} &= \mathbf{W}\mathbf{x} + \mathbf{b} \\
\mathbf{y} &= \mathrm{softmax}(\mathbf{z}) \\
\mathcal{L}_{\mathrm{CE}} &= -\mathbf{t}^{\top}(\log \mathbf{y})
\end{aligned}
$$

- Gradient descent updates are derived in the readings:

$$
\frac{\partial \mathcal{L}_{\mathrm{CE}}}{\partial \mathbf{z}} = \mathbf{y} - \mathbf{t}
$$

Questions?

?

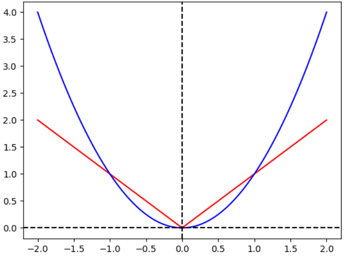
Today's Agenda

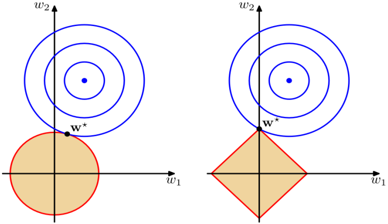
Today's agenda:

- Optimization
  - choice of learning rate
  - stochastic gradient descent
- Multiclass classification
  - softmax regression
- L^1 **regularization**
- Support vector machines
- Boosting

L^1 vs. L^2 Regularization

- The L^1 norm, or sum of absolute values, is another regularizer that encourages weights to be exactly zero. (How can you tell?)
- We can design regularizers based on whatever property we'd like to encourage.





L2 regularization

$$\mathcal{R} = \sum_i w_i^2$$

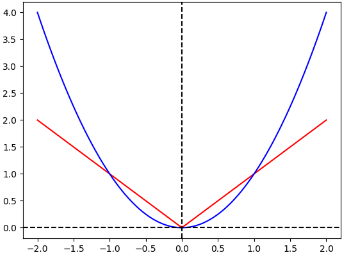
L1 regularization

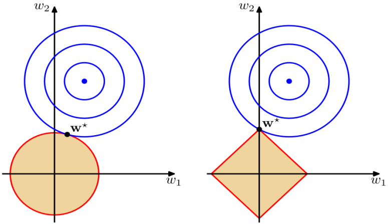
$$\mathcal{R} = \sum_i |w_i|$$

— Bishop, *Pattern Recognition and Machine Learning*

L^1 vs. L^2 Regularization

- The L^1 norm, or sum of absolute values, is another regularizer that encourages weights to be exactly zero. (How can you tell?)
- We can design regularizers based on whatever property we'd like to encourage.
  - Which one will more strongly penalize very large weights?





L2 regularization

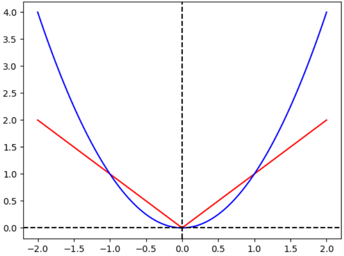
$$\mathcal{R} = \sum_i w_i^2$$

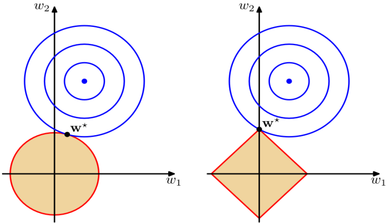
L1 regularization

$$\mathcal{R} = \sum_i |w_i|$$

— Bishop, *Pattern Recognition and Machine Learning*

- The L^1 norm, or sum of absolute values, is another regularizer that encourages weights to be exactly zero. (How can you tell?)
- We can design regularizers based on whatever property we'd like to encourage.
  - Which one will more strongly penalize very large weights?
  - Which one will try harder to push small weights towards zero?





L2 regularization

$$\mathcal{R} = \sum_i w_i^2$$

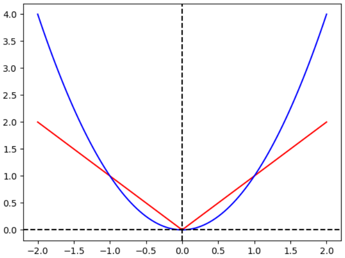
L1 regularization

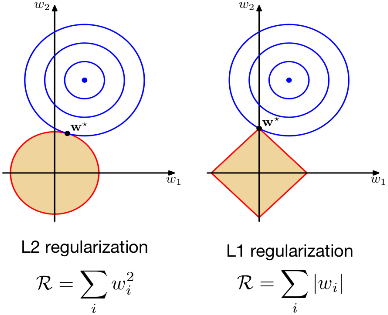
$$\mathcal{R} = \sum_i |w_i|$$

— Bishop, *Pattern Recognition and Machine Learning*

L^1 vs. L^2 Regularization

- The L^1 norm, or sum of absolute values, is another regularizer that encourages weights to be exactly zero. (How can you tell?)
- We can design regularizers based on whatever property we'd like to encourage.
  - Which one will more strongly penalize very large weights?
  - Which one will try harder to push small weights towards zero?
- The derivative at a given value of w_i determines how hard the regularizer "pushes."





— Bishop, *Pattern Recognition and Machine Learning*

L^1 vs. L^2 Regularization

- L^1-regularized linear regression:

$$\mathcal{J}(\mathbf{w}) = \frac{1}{2N} \sum_{i=1}^{N} (\mathbf{w}^\top \mathbf{x}^{(i)} - t^{(i)})^2 \; + \; \lambda \sum_{j=1}^{D} |w_j|$$

- What happens when λ is very large?

L^1 vs. L^2 Regularization

- L^1-regularized linear regression:

$$\mathcal{J}(\mathbf{w}) = \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{w}^\top \mathbf{x}^{(i)} - t^{(i)})^2 \; + \; \lambda \sum_{j=1}^{D} |w_j|$$

- What happens when λ is very large?
- In general, the optimal weight vector will be sparse, i.e. many of the weights will be exactly zero.
    - This is useful in situations where you have lots of features, but only a small fraction of them are likely to be relevant (e.g. genetics).

L^1 vs. L^2 Regularization

- L^1-regularized linear regression:

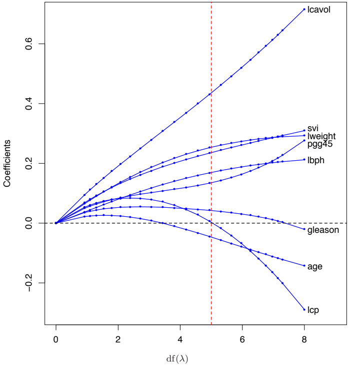
$$\mathcal{J}(\mathbf{w}) = \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{w}^\top \mathbf{x}^{(i)} - t^{(i)})^2 \; + \; \lambda \sum_{j=1}^{D} |w_j|$$

- What happens when λ is very large?
- In general, the optimal weight vector will be sparse, i.e. many of the weights will be exactly zero.
  - This is useful in situations where you have lots of features, but only a small fraction of them are likely to be relevant (e.g. genetics).
- The above cost function is a quadratic program, a more difficult optimization problem than for L^2 regularization.
  - Fast algorithms are implemented in frameworks like scikit-learn.

L^1 vs. L^2 Regularization

- How the linear regression weights evolve for L^2 and L^1 regularization, as a function of the regularization parameter λ.
  - λ *decreases* as you move to the right.

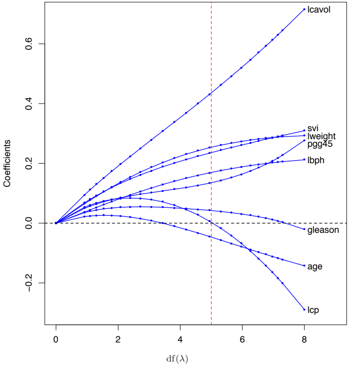
L^2 regularization



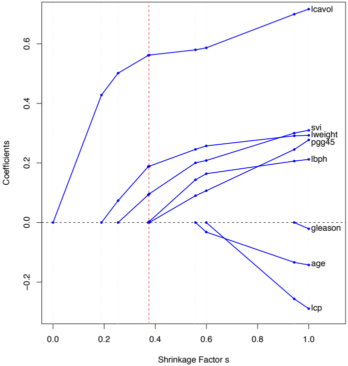
L^1 vs. L^2 Regularization

- How the linear regression weights evolve for L^2 and L^1 regularization, as a function of the regularization parameter λ.
  - λ *decreases* as you move to the right.

L^2 regularization



L^1 regularization



— *Elements of Statistical Learning*

Questions?

?

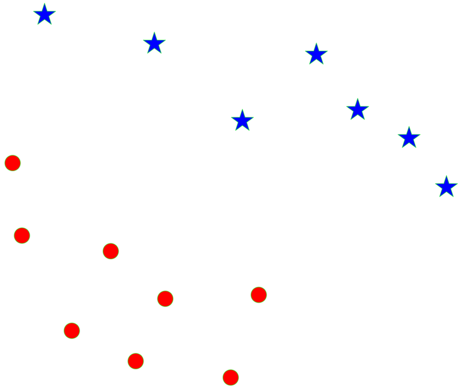
Today's Agenda

Today's agenda:

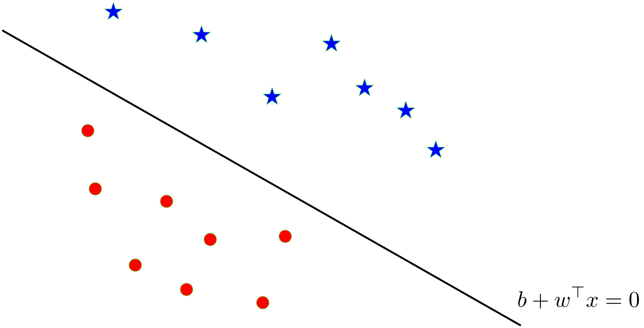
- Optimization
  - choice of learning rate
  - stochastic gradient descent
- Multiclass classification
  - softmax regression
- L^1 regularization
- **Support vector machines**
- Boosting

Separating Hyperplanes

Suppose we are given these data points from two different classes and want to find a linear classifier that separates them.

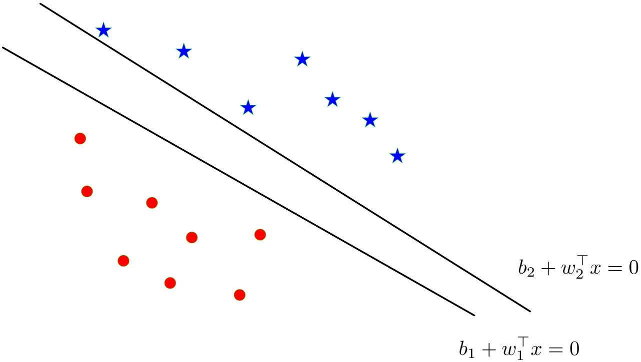


Separating Hyperplanes



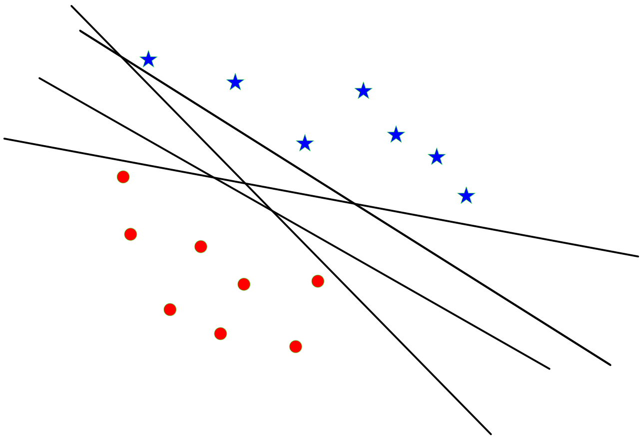
- The decision boundary looks like a line because $\mathbf{x} \in \mathbb{R}^2$, but think about it as a $D-1$ dimensional hyperplane.
- Recall that a hyperplane is described by points $\mathbf{x} \in \mathbb{R}^D$ such that $f(\mathbf{x}) = \mathbf{w}^\top x + b = 0$.

Separating Hyperplanes



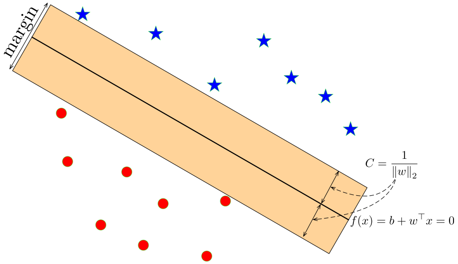
- There are multiple separating hyperplanes, described by different parameters $(\mathbf{w}, b)$.

Separating Hyperplanes



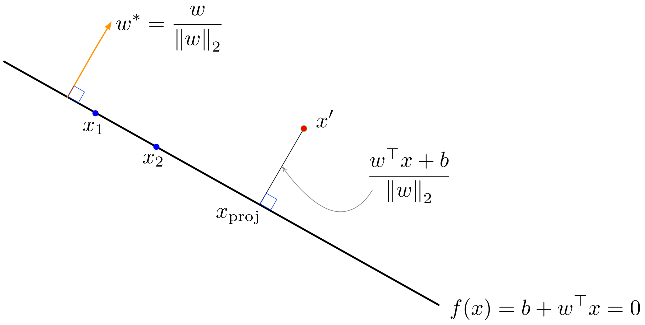
Optimal Separating Hyperplane

Optimal Separating Hyperplane: A hyperplane that separates two classes and maximizes the distance to the closest point from either class, i.e., maximize the margin of the classifier.



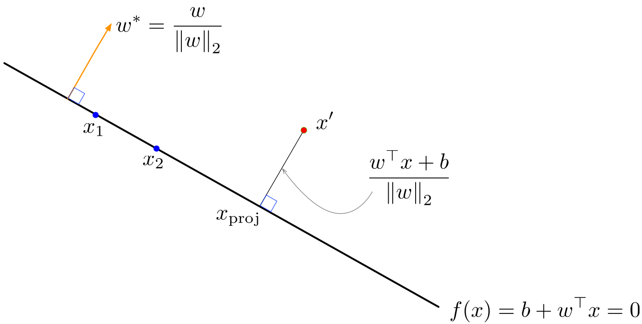
Intuitively, ensuring that a classifier is not too close to any data points leads to better generalization on the test data.

Geometry of Points and Planes



- Recall that the decision hyperplane is orthogonal (perpendicular) to $\mathbf{w}$.
- The vector $\mathbf{w}^* = \frac{\mathbf{w}}{\|\mathbf{w}\|_2}$ is a unit vector pointing in the same direction as $\mathbf{w}$.
- The same hyperplane could equivalently be defined in terms of $\mathbf{w}^*$.

Geometry of Points and Planes



The signed distance of a point $\mathbf{x}'$ to the hyperplane is

$$\frac{\mathbf{w}^\top \mathbf{x}' + b}{\|\mathbf{w}\|_2}$$

Maximizing Margin as an Optimization Problem

- Recall: the classification for the *i*-th data point is correct when

$$\text{sign}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) = t^{(i)}$$

- This can be rewritten as

$$t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) > 0$$

Maximizing Margin as an Optimization Problem

- Recall: the classification for the *i*-th data point is correct when

$$\text{sign}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) = t^{(i)}$$

- This can be rewritten as

$$t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) > 0$$

- Enforcing a margin of C:

$$t^{(i)} \cdot \underbrace{\frac{(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2}}_{\text{signed distance}} \geq C$$

Maximizing Margin as an Optimization Problem

Max-margin objective:

$$\max_{\mathbf{w},b} C$$

$$\text{s.t. } \frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq C \qquad i = 1, \ldots, N$$

Maximizing Margin as an Optimization Problem

Max-margin objective:

$$\max_{\mathbf{w},b} C$$

$$\text{s.t.} \ \frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq C \qquad i = 1, \dots, N$$

Plug in $C = 1/\|\mathbf{w}\|_2$ and simplify:

$$\underbrace{\frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq \frac{1}{\|\mathbf{w}\|_2}}_{\text{geometric margin constraint}} \qquad \iff \qquad \underbrace{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1}_{\text{algebraic margin constraint}}$$

Maximizing Margin as an Optimization Problem

Max-margin objective:

$$\max_{\mathbf{w},b} C$$
$$\text{s.t. } \frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq C \qquad i = 1, \ldots, N$$

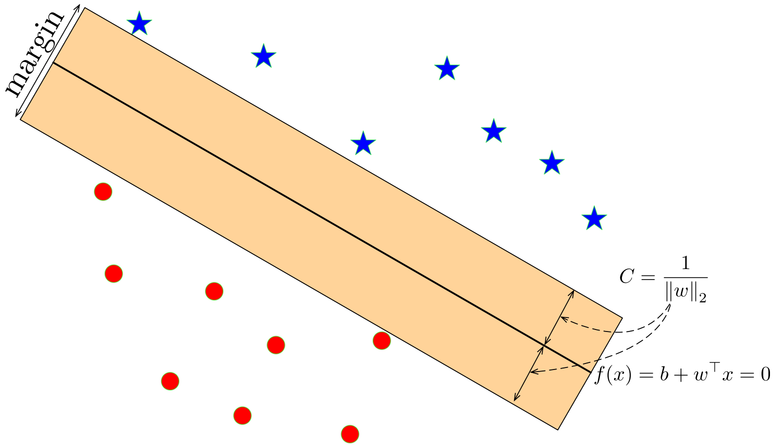
Plug in $C = 1/\|\mathbf{w}\|_2$ and simplify:

$$\underbrace{\frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq \frac{1}{\|\mathbf{w}\|_2}}_{\text{geometric margin constraint}} \qquad \iff \qquad \underbrace{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1}_{\text{algebraic margin constraint}}$$

Equivalent optimization objective:

$$\min \|\mathbf{w}\|_2^2$$
$$\text{s.t. } t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 \qquad i = 1, \ldots, N$$

Maximizing Margin as an Optimization Problem

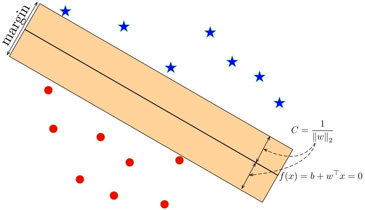


Maximizing Margin as an Optimization Problem

Algebraic max-margin objective:

$$\min_{\mathbf{w},b} \|\mathbf{w}\|_2^2$$

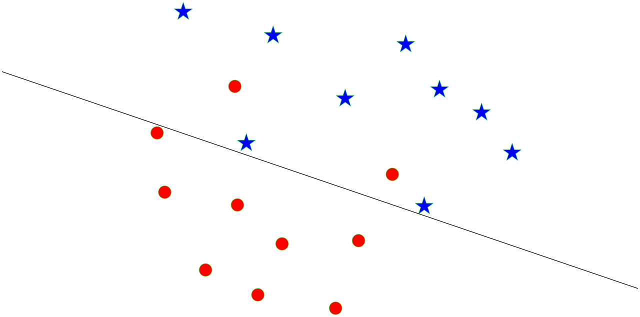
$$\text{s.t.} \;\; t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 \qquad i = 1, \dots, N$$



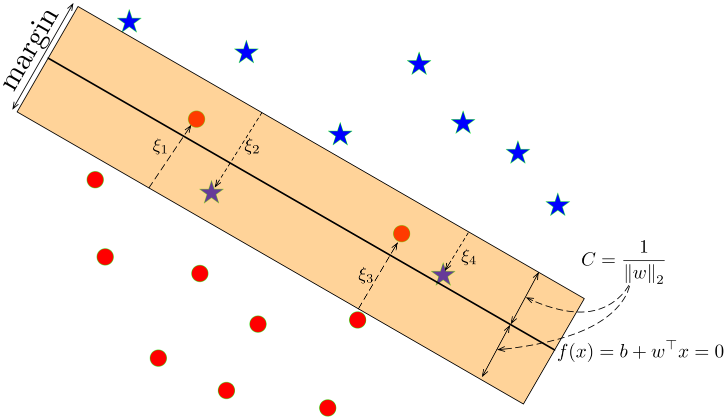
- Observe: if the margin constraint is not tight for $\mathbf{x}^{(i)}$, we could remove it from the training set and the optimal $\mathbf{w}$ would be the same.
- The important training examples are the ones with algebraic margin 1, and are called support vectors.
- Hence, this algorithm is called the (hard) Support Vector Machine (SVM) (or Support Vector Classifier).
- SVM-like algorithms are often called max-margin or large-margin.

Non-Separable Data Points

How can we apply the max-margin principle if the data are **not** linearly separable?



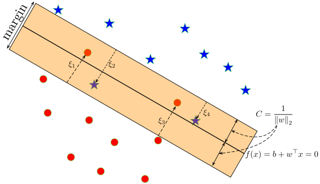
Maximizing Margin for Non-Separable Data Points



Main Idea:

- Allow some points to be within the margin or even be misclassified; we represent this with slack variables ξ_i.
- But constrain or penalize the total amount of slack.

Maximizing Margin for Non-Separable Data Points



- Soft margin constraint:

$$\frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq C(1 - \xi_i),$$

  for $\xi_i \geq 0$.
- Penalize $\sum_i \xi_i$

Maximizing Margin for Non-Separable Data Points

Soft-margin SVM objective:

$$
\begin{aligned}
\min_{\mathbf{w},b,\xi} \; & \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_{i=1}^{N} \xi_i \\
\text{s.t.} \quad & t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 - \xi_i \qquad i = 1, \ldots, N \\
& \xi_i \geq 0 \qquad i = 1, \ldots, N
\end{aligned}
$$

Maximizing Margin for Non-Separable Data Points

Soft-margin SVM objective:

$$\begin{aligned}
&\min_{\mathbf{w},b,\xi} \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_{i=1}^{N} \xi_i \\
\text{s.t.} \quad & t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 - \xi_i \qquad i = 1, \ldots, N \\
& \xi_i \geq 0 \qquad\qquad\qquad\qquad\quad i = 1, \ldots, N
\end{aligned}$$

- γ is a hyperparameter that trades off the margin with the amount of slack.
  - For $\gamma = 0$, we'll get $\mathbf{w} = 0$. (Why?)
  - As $\gamma \to \infty$ we get the hard-margin objective.
- Note: it is also possible to constrain $\sum_i \xi_i$ instead of penalizing it.

From Margin Violation to Hinge Loss

Let's simplify the soft margin constraint by eliminating ξ_i. Recall:

$$
\begin{aligned}
t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) &\geq 1 - \xi_i \qquad && i = 1, \ldots, N \\
\xi_i &\geq 0 && i = 1, \ldots, N
\end{aligned}
$$

- Rewrite as $\xi_i \geq 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)$.

From Margin Violation to Hinge Loss

Let's simplify the soft margin constraint by eliminating ξ_i. Recall:

$$t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 - \xi_i \qquad i = 1, \ldots, N$$
$$\xi_i \geq 0 \qquad i = 1, \ldots, N$$

- Rewrite as $\xi_i \geq 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)$.
- **Case 1:** $1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \leq 0$
  - The smallest non-negative ξ_i that satisfies the constraint is $\xi_i = 0$.
- **Case 2:** $1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) > 0$
  - The smallest ξ_i that satisfies the constraint is $\xi_i = 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)$.
- Hence, $\xi_i = \max\{0, 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)\}$.

From Margin Violation to Hinge Loss

Let's simplify the soft margin constraint by eliminating ξ_i. Recall:

$$\begin{aligned} t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) &\geq 1 - \xi_i \qquad & i = 1, \dots, N \\ \xi_i &\geq 0 & i = 1, \dots, N \end{aligned}$$

- Rewrite as $\xi_i \geq 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)$.
- **Case 1:** $1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \leq 0$
  - The smallest non-negative ξ_i that satisfies the constraint is $\xi_i = 0$.
- **Case 2:** $1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) > 0$
  - The smallest ξ_i that satisfies the constraint is $\xi_i = 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)$.
- Hence, $\xi_i = \max\{0, 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)\}$.
- Therefore, the slack penalty can be written as

$$\sum_{i=1}^{N} \xi_i = \sum_{i=1}^{N} \max\{0, 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)\}.$$

- We sometimes write $\max\{0, y\} = (y)_+$

From Margin Violation to Hinge Loss

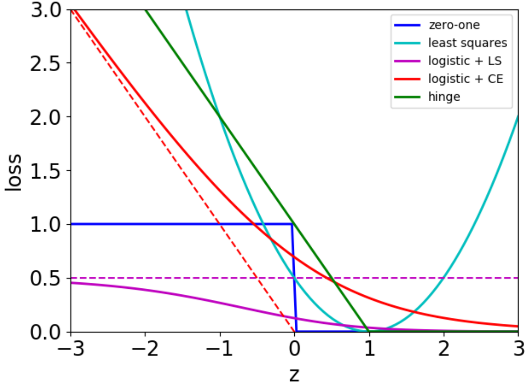
If we write $y^{(i)}(\mathbf{w}, b) = \mathbf{w}^\top \mathbf{x} + b$, then the optimization problem can be written as

$$\min_{\mathbf{w},b,\xi} \sum_{i=1}^{N} \left(1 - t^{(i)} y^{(i)}(\mathbf{w}, b)\right)_+ + \frac{1}{2\gamma} \|\mathbf{w}\|_2^2$$

- The loss function $\mathcal{L}_{\mathrm{H}}(y, t) = (1 - ty)_+$ is called the hinge loss.
- The second term is the L_2-norm of the weights.
- Hence, the soft-margin SVM can be seen as a linear classifier with hinge loss and an L_2 regularizer.

Revisiting Loss Functions for Classification

Hinge loss compared with other loss functions



SVMs: What we Left Out

What we left out:

- How to fit $\mathbf{w}$:
  - One option: gradient descent
  - Can reformulate with the Lagrange dual
- The "kernel trick" converts it into a powerful nonlinear classifier. This is covered in CSC2506 and CSC2547.
- Classic results from learning theory show that a large margin implies good generalization.

Questions?

?

Today's Agenda

Today's agenda:

- Optimization
  - choice of learning rate
  - stochastic gradient descent
- Multiclass classification
  - softmax regression
- L^1 regularization
- Support vector machines
- **Boosting**

Boosting

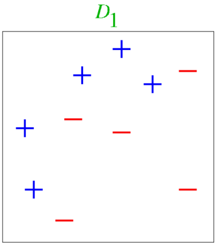
- Recall that an *ensemble* is a set of predictors whose individual decisions are combined in some way to classify new examples.
- (Lecture 2) **Bagging**: Train classifiers independently on random subsets of the training data.
- (This lecture) **Boosting**: Train classifiers sequentially, each time focusing on training data points that were previously misclassified.
- Let us start with the concept of weak learner/classifier (or base classifiers).

Weak Learner/Classifier

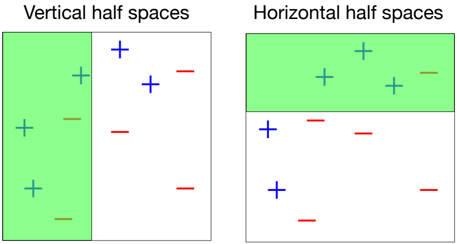
- (Informal) Weak learner is a learning algorithm that outputs a hypothesis (e.g., a classifier) that performs slightly better than chance, e.g., it predicts the correct label with probability 0.6.
- We are interested in weak learners that are *computationally* efficient.
  - Decision trees
  - Even simpler: Decision Stump: A decision tree with only a single split

[Formal definition of weak learnability has quantifies such as "for any distribution over data" and the requirement that its guarantee holds only probabilistically.]

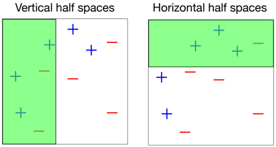
Weak Classifiers



These weak classifiers, which are decision stumps, consist of the set of horizontal and vertical half spaces.



Weak Classifiers



- A *single* weak classifier is not capable of making the training error very small. It only perform slightly better than chance, i.e., the error of classifier h according to the given weights $\mathbf{w} = (w_1, \ldots, w_N)$ (with $\sum_{i=1}^N w_i = 1$ and $w_i \geq 0$)

$$\text{err} = \sum_{i=1}^{N} w_i \mathbb{I}\{h(\mathbf{x}_i) \neq y_i\}$$

  is at most $\frac{1}{2} - \gamma$ for some $\gamma > 0$.

- Can we combine a set of weak classifiers in order to make a better ensemble of classifiers?

- Boosting: Train classifiers sequentially, each time focusing on training data points that were previously misclassified.

AdaBoost (Adaptive Boosting)

- Key steps of AdaBoost:
  1. At each iteration we re-weight the training samples by assigning larger weights to samples (i.e., data points) that were classified incorrectly.
  2. We train a new weak classifier based on the re-weighted samples.
  3. We add this weak classifier to the ensemble of classifiers. This is our new classifier.
  4. We repeat the process many times.

AdaBoost (Adaptive Boosting)

- Key steps of AdaBoost:
  1. At each iteration we re-weight the training samples by assigning larger weights to samples (i.e., data points) that were classified incorrectly.
  2. We train a new weak classifier based on the re-weighted samples.
  3. We add this weak classifier to the ensemble of classifiers. This is our new classifier.
  4. We repeat the process many times.
- The weak learner needs to minimize weighted error.

AdaBoost (Adaptive Boosting)

- Key steps of AdaBoost:
  1. At each iteration we re-weight the training samples by assigning larger weights to samples (i.e., data points) that were classified incorrectly.
  2. We train a new weak classifier based on the re-weighted samples.
  3. We add this weak classifier to the ensemble of classifiers. This is our new classifier.
  4. We repeat the process many times.
- The weak learner needs to minimize weighted error.
- AdaBoost reduces bias by making each classifier focus on previous mistakes.

AdaBoost Example

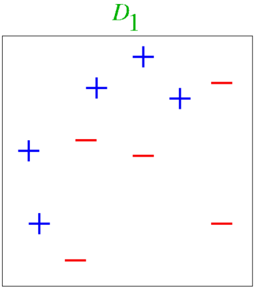
- ϵ_t is the weighted error, assuming less than $1/2$.
- $\alpha_t = \frac{1}{2}\log(\frac{1-\epsilon_t}{\epsilon_t})$ measures the classifier quality.
- Weight the binary prediction of each classifier by the quality of that classifier:

$$H(\mathbf{x}) = \text{sign}(F(\mathbf{x})) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m y_m(\mathbf{x})\right)$$

- This is how to do inference, i.e., how to compute the prediction for each new example.

AdaBoost Example

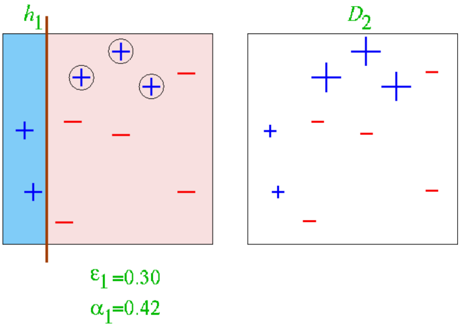
- Training data



[Slide credit: Verma & Thrun]

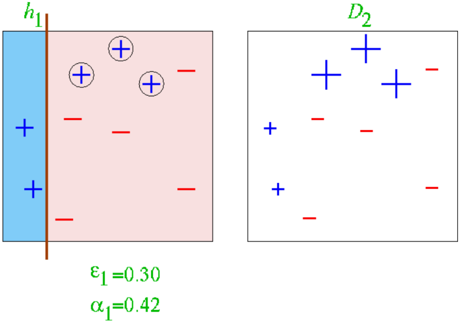
AdaBoost Example

- Round 1



AdaBoost Example

- Round 1



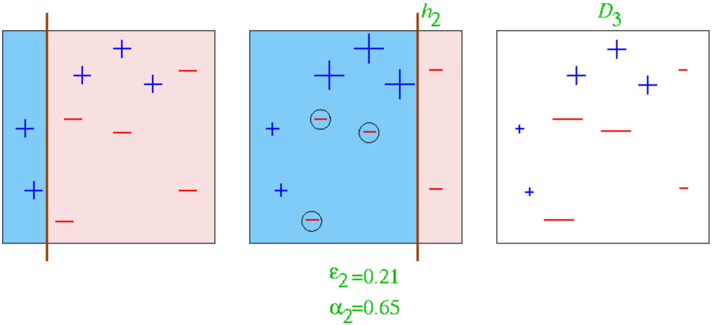
$$\mathbf{w} = \left(\frac{1}{10}, \ldots, \frac{1}{10}\right) \Rightarrow \text{Train a classifier (using } \mathbf{w}\text{)} \Rightarrow \text{err}_1 = \frac{\sum_{i=1}^{10} w_i \mathbb{I}\{h_1(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^{N} w_i} = \frac{3}{10}$$

$$\Rightarrow \alpha_1 = \frac{1}{2} \log \frac{1 - \text{err}_1}{\text{err}_1} = \frac{1}{2} \log(\frac{1}{0.3} - 1) \approx 0.42 \Rightarrow H(\mathbf{x}) = \text{sign}\left(\alpha_1 h_1(\mathbf{x})\right)$$

[Slide credit: Verma & Thrun]

AdaBoost Example

- Round 2



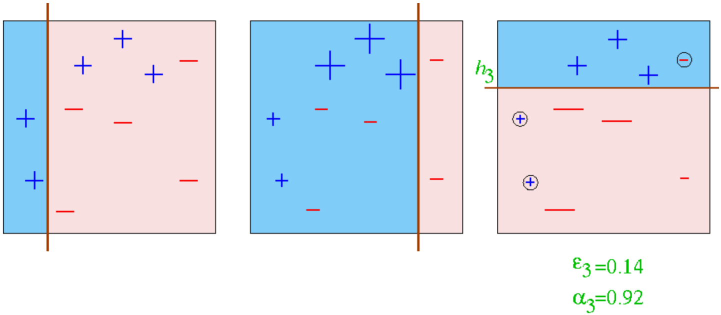
$$\mathbf{w} = \text{updated weights} \Rightarrow \text{Train a classifier (using } \mathbf{w}) \Rightarrow \text{err}_2 = \frac{\sum_{i=1}^{10} w_i \mathbb{I}\{h_2(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^{N} w_i} = 0.21$$

$$\Rightarrow \alpha_2 = \frac{1}{2} \log \frac{1 - \text{err}_3}{\text{err}_3} = \frac{1}{2} \log(\frac{1}{0.21} - 1) \approx 0.66 \Rightarrow H(\mathbf{x}) = \text{sign}\left(\alpha_1 h_1(\mathbf{x}) + \alpha_2 h_2(\mathbf{x})\right)$$

[Slide credit: Verma & Thrun]

AdaBoost Example

- Round 3



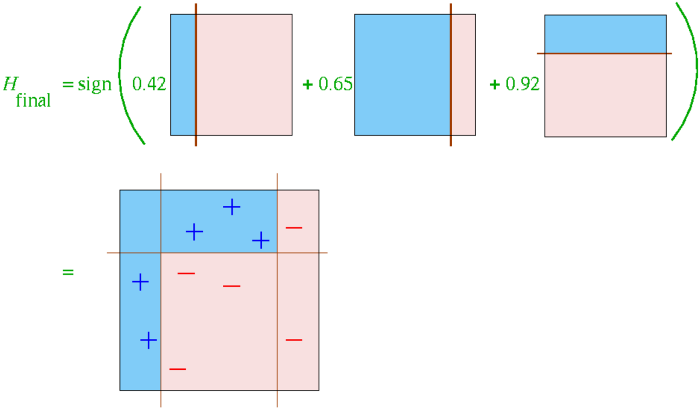
$$\mathbf{w} = \text{updated weights} \Rightarrow \text{Train a classifier (using } \mathbf{w}) \Rightarrow \text{err}_3 = \frac{\sum_{i=1}^{10} w_i \mathbb{I}\{h_3(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^{N} w_i} = 0.14$$

$$\Rightarrow \alpha_3 = \frac{1}{2}\log\frac{1-\text{err}_3}{\text{err}_3} = \frac{1}{2}\log(\frac{1}{0.14} - 1) \approx 0.91 \Rightarrow H(\mathbf{x}) = \text{sign}\left(\alpha_1 h_1(\mathbf{x}) + \alpha_2 h_2(\mathbf{x}) + \alpha_3 h_3(\mathbf{x})\right)$$

[Slide credit: Verma & Thrun]

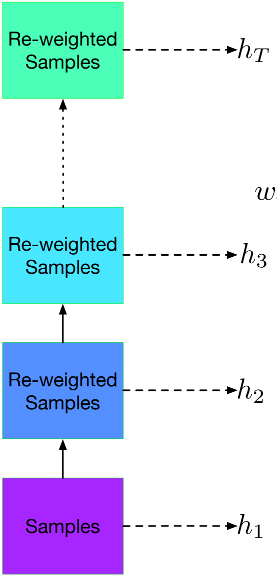
AdaBoost Example

- Final classifier



[Slide credit: Verma & Thrun]

AdaBoost Algorithm



$$H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

$$w_i \leftarrow w_i \exp\left(2\alpha_t \mathbb{I}\{h_t(\mathbf{x}^{(\mathbf{i})}) \neq \mathbf{t}^{(\mathbf{i})}\}\right)$$

$$\alpha_t = \frac{1}{2}\log\left(\frac{1-\text{err}_t}{\text{err}_t}\right)$$

$$\text{err}_t = \frac{\sum_{i=1}^{N} w_i \mathbb{I}\{h_t(\mathbf{x}^{(\mathbf{i})} \neq \mathbf{t}^{(\mathbf{i})}\}}{\sum_{i=1}^{N} w_i}$$

AdaBoost Algorithm

- Input: Data $\mathcal{D}_N = \{\mathbf{x}^{(i)}, t^{(i)}\}_{i=1}^{N}$, weak classifier WeakLearn (a classification procedure that return a classifier from base hypothesis space $\mathcal{H}$ with $h : \mathbf{x} \rightarrow \{-1, +1\}$ for $h \in \mathcal{H}$), number of iterations T
- Output: Classifier $H(x)$
- Initialize sample weights: $w_i = \frac{1}{N}$ for $i = 1, \dots, N$
- For $t = 1, \dots, T$
  - Fit a classifier to data using weighted samples ($h_t \leftarrow \mathit{WeakLearn}(\mathcal{D}_N, \mathbf{w})$), e.g.,

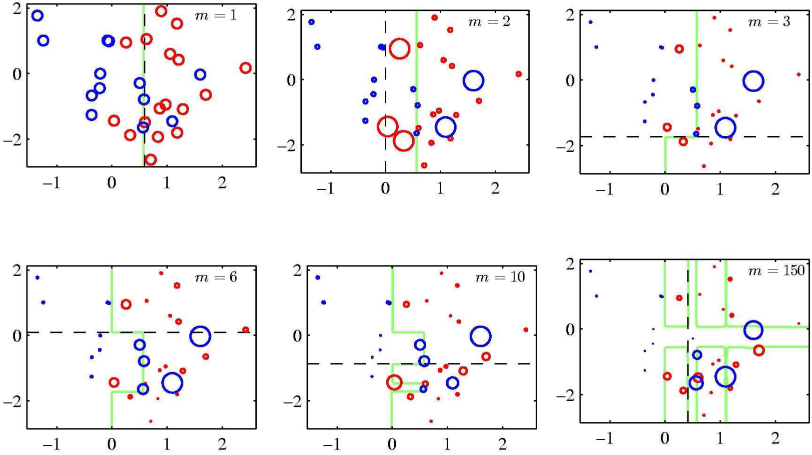
$$h_t \leftarrow \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{N} w_i \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t^{(i)}\}$$

  - Compute weighted error $\mathrm{err}_t = \frac{\sum_{i=1}^{N} w_i \mathbb{I}\{h_t(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^{N} w_i}$
  - Compute classifier coefficient $\alpha_t = \frac{1}{2} \log \frac{1 - \mathrm{err}_t}{\mathrm{err}_t}$
  - Update data weights

$$w_i \leftarrow w_i \exp\left(-\alpha_t t^{(i)} h_t(\mathbf{x}^{(i)})\right) \left[\equiv w_i \exp\left(2\alpha_t \mathbb{I}\{h_t(\mathbf{x}^{(i)}) \neq t^{(i)}\}\right)\right]$$

- Return $H(\mathbf{x}) = \mathrm{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right)$

AdaBoost Example



- Each figure shows the number m of base learners trained so far, the decision of the most recent learner (dashed black), and the boundary of the ensemble (green)

AdaBoost Minimizes the Training Error

Theorem

Assume that at each iteration of AdaBoost the WeakLearn returns a hypothesis with error $\text{err}_t \leq \frac{1}{2} - \gamma$ for all $t = 1, \ldots, T$ with $\gamma > 0$. The training error of the output hypothesis $H(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right)$ is at most

$$L_N(H) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}\{H(\mathbf{x}^{(i)}) \neq t^{(i)})\} \leq \exp\left(-2\gamma^2 T\right).$$

AdaBoost Minimizes the Training Error

Theorem

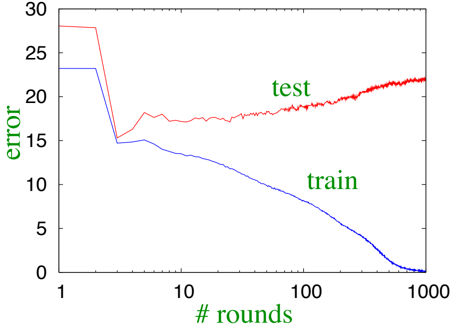
Assume that at each iteration of AdaBoost the WeakLearn returns a hypothesis with error $\text{err}_t \leq \frac{1}{2} - \gamma$ for all $t = 1, \ldots, T$ with $\gamma > 0$. The training error of the output hypothesis $H(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right)$ is at most

$$L_N(H) = \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}\{H(\mathbf{x}^{(i)}) \neq t^{(i)})\} \leq \exp\left(-2\gamma^2 T\right).$$

- This is under the simplifying assumption that each weak learner is γ-better than a random predictor.
- Maybe this assumption is less innocuous than it seems.

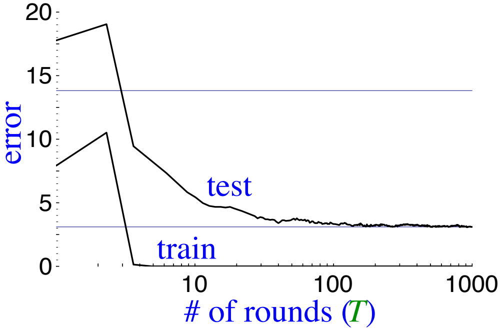
Generalization Error of AdaBoost

- AdaBoost's training error (loss) converges to zero. What about the test error of H?
- As we add more weak classifiers, the overall classifier H becomes more "complex".
- We expect more complex classifiers overfit.
- If one runs AdaBoost long enough, it can in fact overfit.



Generalization Error of AdaBoost

- But often it does not!
- Sometimes the test error decreases even after the training error is zero!



[Slide credit: Robert Shapire's Slides, `http://www.cs.princeton.edu/courses/archive/spring12/cos598A/schedule.html`]

Additive Models

- Consider a hypothesis class $\mathcal{H}$ with each $h_i : \mathbf{x} \mapsto \{-1, +1\}$ within $\mathcal{H}$, i.e., $h_i \in \mathcal{H}$. These are the "weak learners", and in this context they're also called bases.
- An additive model with m terms is given by

$$H_m(x) = \sum_{i=1}^{m} \alpha_i h_i(\mathbf{x}),$$

  where $(\alpha_1, \cdots, \alpha_m) \in \mathbb{R}^m$.
- Observe that we're taking a linear combination of base classifiers, just like in boosting.
- We'll now interpret AdaBoost as a way of fitting an additive model.

Stagewise Training of Additive Models

A greedy approach to fitting additive models, known as stagewise training:

1. Initialize $H_0(x) = 0$
2. For $m = 1$ to T:
    - Compute the m-th hypothesis and its coefficient

$$(h_m, \alpha_m) \leftarrow \underset{h \in \mathcal{H}, \alpha}{\operatorname{argmin}} \sum_{i=1}^{N} \mathcal{L}\left(H_{m-1}(\mathbf{x}^{(i)}) + \alpha h(\mathbf{x}^{(i)}), t^{(i)}\right)$$

    - Add it to the additive model

$$H_m = H_{m-1} + \alpha_m h_m$$

AdaBoost as an Additive Models with Exponential Loss

AdaBoost can be derived as an additive model $H_m(x) = \sum_{i=1}^{m} \alpha_i h_i(\mathbf{x})$ with

$$h_m \leftarrow \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\},$$

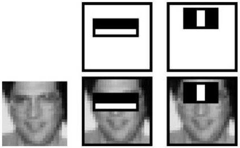
$$\alpha = \frac{1}{2} \log \left(\frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \right), \qquad \text{where } \mathrm{err}_m = \frac{\sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h_m(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^{N} w_i^{(m)}},$$

$$w_i^{(m+1)} = w_i^{(m)} \exp\left(-\alpha_m h_m(\mathbf{x}^{(i)}) t^{(i)} \right).$$

Full derivation for AdaBoost algorithm in Boosting: foundations and algorithms by Robert E. Schapire and Yoav Freund.

AdaBoost for Face Recognition

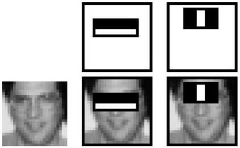
- Viola and Jones (2001) created a very fast face detector that can be scanned across a large image to find the faces.



- The base classifier/weak learner just compares the total intensity in two rectangular pieces of the image.

AdaBoost for Face Recognition

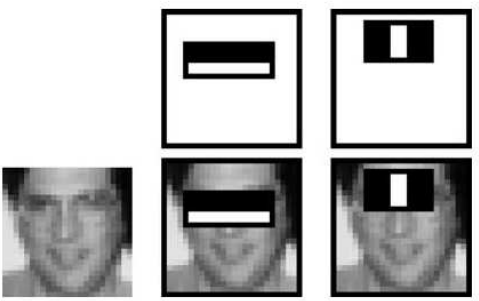
- Viola and Jones (2001) created a very fast face detector that can be scanned across a large image to find the faces.



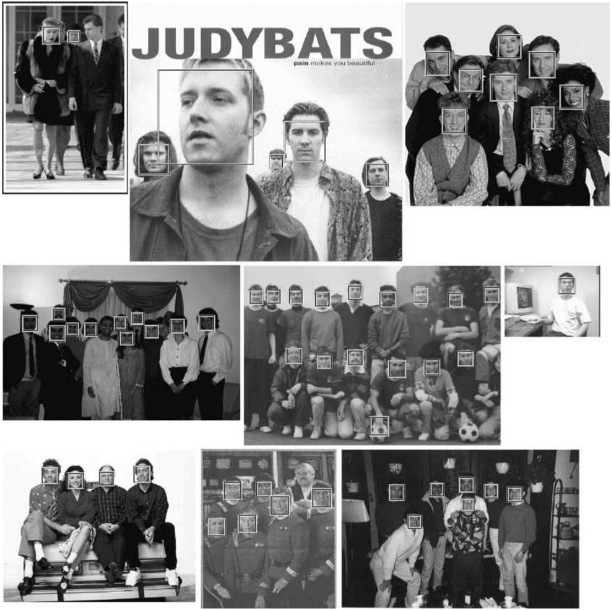
- The base classifier/weak learner just compares the total intensity in two rectangular pieces of the image.
  - There is a neat trick for computing the total intensity in a rectangle in a few operations.
    - So it is easy to evaluate a huge number of base classifiers and they are very fast at runtime.
  - The algorithm adds classifiers greedily based on their quality on the weighted training cases.

AdaBoost for Face Detection

- A few twists on standard algorithm
  - Pre-define weak classifiers, so optimization=selection
  - Change loss function for weak learners: false positives less costly than misses
  - Smart way to do inference in real-time (in 2001 hardware)



AdaBoost Face Detection Results



Questions?

?