# CSC 311: Introduction to Machine Learning <br> Lecture 3 - Bagging, Linear Models I 

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## Today

- Today we will introduce ensembling methods that combine multiple models and can perform better than the individual members.
- We've seen many individual models (KNN, decision trees)
- We will see bagging:
- Train models independently on random "resamples" of the training data.
- We will introduce linear regression, our first parametric learning algorithm.
- This will exemplify how we'll think about learning algorithms for the rest of the course.


## Bias/Variance Decomposition

- Recall, we treat predictions $y$ at a query $\mathbf{x}$ as a random variable (where the randomness comes from the choice of dataset), $y_{\star}$ is the optimal deterministic prediction, $t$ is a random target sampled from the true conditional $p(t \mid \mathbf{x})$.

$$
\mathbb{E}\left[(y-t)^{2}\right]=\underbrace{\left(y_{\star}-\mathbb{E}[y]\right)^{2}}_{\text {bias }}+\underbrace{\operatorname{Var}(y)}_{\text {variance }}+\underbrace{\operatorname{Var}(t)}_{\text {Bayes error }}
$$

- Bias/variance decomposes the expected loss into three terms:
- bias: how wrong the expected prediction is (corresponds to underfitting)
- variance: the amount of variability in the predictions (corresponds to overfitting)
- Bayes error: the inherent unpredictability of the targets
- Even though this analysis only applies to squared error, we often loosely use "bias" and "variance" as synonyms for "underfitting" and "overfitting".


## Bias/Variance Decomposition: Another Visualization

- We can visualize this decomposition in output space, where the axes correspond to predictions on the test examples.
- If we have an overly simple model (e.g. KNN with large $k$ ), it might have
- high bias (because it cannot capture the structure in the data)
- low variance (because there's enough data to get stable estimates)



## Bias/Variance Decomposition: Another Visualization

- If you have an overly complex model (e.g. KNN with $k=1$ ), it might have
- low bias (since it learns all the relevant structure)
- high variance (it fits the quirks of the data you happened to sample)



## Bias/Variance Decomposition: Another Visualization

- The following graphic summarizes the previous two slides:

- What doesn't this capture?


## Bagging: Motivation

- Suppose we could somehow sample $m$ independent training sets from $p_{\text {sample }}$.
- We could then compute the prediction $y_{i}$ based on each one, and take the average $y=\frac{1}{m} \sum_{i=1}^{m} y_{i}$.
- How does this affect the three terms of the expected loss?
- Bayes error: unchanged, since we have no control over it
- Bias: unchanged, since the averaged prediction has the same expectation

$$
\mathbb{E}[y]=\mathbb{E}\left[\frac{1}{m} \sum_{i=1}^{m} y_{i}\right]=\mathbb{E}\left[y_{i}\right]
$$

- Variance: reduced, since we're averaging over independent samples

$$
\operatorname{Var}[y]=\operatorname{Var}\left[\frac{1}{m} \sum_{i=1}^{m} y_{i}\right]=\frac{1}{m^{2}} \sum_{i=1}^{m} \operatorname{Var}\left[y_{i}\right]=\frac{1}{m} \operatorname{Var}\left[y_{i}\right]
$$

## Bagging: The Idea

- In practice, the sampling distribution $p_{\text {sample }}$ is often finite or expensive to sample from.
- So training separate models on independently sampled datasets is very wasteful of data!
- Why not train a single model on the union of all sampled datasets?
- Solution: given training set $\mathcal{D}$, use the empirical distribution $p_{\mathcal{D}}$ as a proxy for $p_{\text {sample }}$. This is called bootstrap aggregation, or bagging .
- Take a single dataset $\mathcal{D}$ with $n$ examples.
- Generate $m$ new datasets ("resamples" or "bootstrap samples"), each by sampling $n$ training examples from $\mathcal{D}$, with replacement.
- Average the predictions of models trained on each of these datasets.
- The bootstrap is one of the most important ideas in all of statistics!
- Intuition: As $|\mathcal{D}| \rightarrow \infty$, we have $p_{\mathcal{D}} \rightarrow p_{\text {sample }}$.


## Bagging



## Bagging

$$
\begin{aligned}
& \text { predicting on a query point } x
\end{aligned}
$$

## Bagging for Binary Classification

- If our classifiers output real-valued probabilities, $z_{i} \in[0,1]$, then we can average the predictions before thresholding:

$$
y_{\text {bagged }}=\mathbb{I}\left(z_{\text {bagged }}>0.5\right)=\mathbb{I}\left(\sum_{i=1}^{m} \frac{z_{i}}{m}>0.5\right)
$$

- If our classifiers output binary decisions, $y_{i} \in\{0,1\}$, we can still average the predictions before thresholding:

$$
y_{\text {bagged }}=\mathbb{I}\left(\sum_{i=1}^{m} \frac{y_{i}}{m}>0.5\right)
$$

This is the same as taking a majority vote.

- A bagged classifier can be stronger than the average underyling model.
- E.g., individual accuracy on "Who Wants to be a Millionaire" is only so-so, but "Ask the Audience" is quite effective.


## Bagging: Effect of Correlation

- Problem: the datasets are not independent, so we don't get the $1 / m$ variance reduction.
- Possible to show that if the sampled predictions have variance $\sigma^{2}$ and correlation $\rho$, then

$$
\operatorname{Var}\left(\frac{1}{m} \sum_{i=1}^{m} y_{i}\right)=\frac{1}{m}(1-\rho) \sigma^{2}+\rho \sigma^{2} .
$$

- Ironically, it can be advantageous to introduce additional variability into your algorithm, as long as it reduces the correlation between samples.
- Intuition: you want to invest in a diversified portfolio, not just one stock.
- Can help to use average over multiple algorithms, or multiple configurations of the same algorithm.


## Random Forests

- Random forests $=$ bagged decision trees, with one extra trick to decorrelate the predictions
- When choosing each node of the decision tree, choose a random set of $d$ input features, and only consider splits on those features
- Random forests are probably the best black-box machine learning algorithm - they often work well with no tuning whatsoever.
- one of the most widely used algorithms in Kaggle competitions


## Bagging Summary

- Bagging reduces overfitting by averaging predictions.
- Used in most competition winners
- Even if a single model is great, a small ensemble usually helps.
- Limitations:
- Does not reduce bias in case of squared error.
- There is still correlation between classifiers.
- Random forest solution: Add more randomness.
- Naive mixture (all members weighted equally).
- If members are very different (e.g., different algorithms, different data sources, etc.), we can often obtain better results by using a principled approach to weighted ensembling.


## Linear Regression

## Overview

- Second learning algorithm of the course: linear regression.
- Task: predict scalar-valued targets (e.g. stock prices)
- Architecture: linear function of the inputs
- While KNN was a complete algorithm, linear regression exemplifies a modular approach that will be used throughout this course:
- choose a model describing the relationships between variables of interest
- define a loss function quantifying how bad the fit to the data is
- choose a regularizer saying how much we prefer different candidate models (or explanations of data)
- fit a model that minimizes the loss function and satisfies the constraint/penalty imposed by the regularizer, possibly using an optimization algorithm
- Mixing and matching these modular components give us a lot of new ML methods.


## Supervised Learning Setup



In supervised learning:

- There is input $\mathbf{x} \in \mathcal{X}$, typically a vector of features (or covariates)
- There is target $t \in \mathcal{T}$ (also called response, outcome, output, class)
- Objective is to learn a function $f: \mathcal{X} \rightarrow \mathcal{T}$ such that $t \approx y=f(\mathbf{x})$ based on some data $\mathcal{D}=\left\{\left(\mathbf{x}^{(i)}, t^{(i)}\right)\right.$ for $\left.i=1,2, \ldots, N\right\}$.


## Linear Regression - Model

- Model: In linear regression, we use a linear function of the features $\mathbf{x}=\left(x_{1}, \ldots, x_{D}\right) \in \mathbb{R}^{D}$ to make predictions $y$ of the target value $t \in \mathbb{R}$ :

$$
y=f(\mathbf{x})=\sum_{j} w_{j} x_{j}+b
$$

- $y$ is the prediction
- w is the weights
- $b$ is the bias (or intercept)
- $\mathbf{w}$ and $b$ together are the parameters
- We hope that our prediction is close to the target: $y \approx t$.


## What is Linear? 1 feature vs D features



- If we have only 1 feature:
$y=w x+b$ where $w, x, b \in \mathbb{R}$.
- $y$ is linear in $x$.
- If we have $D$ features:
$y=\mathbf{w}^{\top} \mathbf{x}+b$ where $\mathbf{w}, \mathbf{x} \in \mathbb{R}^{D}$, $b \in \mathbb{R}$
- $y$ is linear in $\mathbf{x}$.

Relation between the prediction $y$ and inputs $\mathbf{x}$ is linear in both cases.

## Linear Regression - Loss Function

- A loss function $\mathcal{L}(y, t)$ defines how bad it is if, for some example $\mathbf{x}$, the algorithm predicts $y$, but the target is actually $t$.
- Squared error loss function:

$$
\mathcal{L}(y, t)=\frac{1}{2}(y-t)^{2}
$$

- $y-t$ is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.
- Cost function: loss function averaged over all training examples

$$
\begin{aligned}
\mathcal{J}(\mathbf{w}, b) & =\frac{1}{2 N} \sum_{i=1}^{N}\left(y^{(i)}-t^{(i)}\right)^{2} \\
& =\frac{1}{2 N} \sum_{i=1}^{N}\left(\mathbf{w}^{\top} \mathbf{x}^{(i)}+b-t^{(i)}\right)^{2}
\end{aligned}
$$

- Terminology varies. Some call "cost" empirical or average loss.


# Vectorization 

## Vectorization

- The prediction for one data point can be computed using a for loop:

$$
\begin{aligned}
& y=b \\
& \text { for } j \text { in range(M): } \\
& \qquad y+=w[j]^{*} \times[j]
\end{aligned}
$$

- Excessive super/sub scripts are hard to work with, and Python loops are slow, so we vectorize algorithms by expressing them in terms of vectors and matrices.

$$
\begin{gathered}
\mathbf{w}=\left(w_{1}, \ldots, w_{D}\right)^{\top} \quad \mathbf{x}=\left(x_{1}, \ldots, x_{D}\right)^{\top} \\
y=\mathbf{w}^{\top} \mathbf{x}+b
\end{gathered}
$$

- This is simpler and executes much faster:

$$
y=n p \cdot \operatorname{dot}(w, x)+b
$$

## Vectorization

Why vectorize?

- The equations, and the code, will be simpler and more readable. Gets rid of dummy variables/indices!
- Vectorized code is much faster
- Cut down on Python interpreter overhead
- Use highly optimized linear algebra libraries (hardware support)
- Matrix multiplication very fast on GPU (Graphics Processing Unit)

Switching in and out of vectorized form is a skill you gain with practice

- Some derivations are easier to do element-wise
- Some algorithms are easier to write/understand using for-loops and vectorize later for performance


## Vectorization

- We can organize all the training examples into a design matrix $\mathbf{X}$ with one row per training example, and all the targets into the target vector $\mathbf{t}$.


## one feature across <br> all training examples

$$
\mathbf{X}=\left(\begin{array}{l}
\mathbf{x}^{(1) \top} \\
\mathbf{x}^{(2) \top} \\
\mathbf{x}^{(3) \top}
\end{array}\right)=\left(\begin{array}{c|c|cc}
8 & 0 & 3 & 0 \\
\hline 6 & -1 & 5 & 3 \\
\hline 2 & 5 & -2 & 8
\end{array}\right) \begin{gathered}
\text { one training } \\
\text { example (vector) }
\end{gathered}
$$

- Computing the predictions for the whole dataset:

$$
\mathbf{X} \mathbf{w}+b \mathbf{1}=\left(\begin{array}{c}
\mathbf{w}^{T} \mathbf{x}^{(1)}+b \\
\vdots \\
\mathbf{w}^{T} \mathbf{x}^{(N)}+b
\end{array}\right)=\left(\begin{array}{c}
y^{(1)} \\
\vdots \\
y^{(N)}
\end{array}\right)=\mathbf{y}
$$

## Vectorization

- Computing the squared error cost across the whole dataset:

$$
\begin{aligned}
& \mathbf{y}=\mathbf{X} \mathbf{w}+b \mathbf{1} \\
& \mathcal{J}=\frac{1}{2 N}\|\mathbf{y}-\mathbf{t}\|^{2}
\end{aligned}
$$

- Sometimes we may use $\mathcal{J}=\frac{1}{2}\|\mathbf{y}-\mathbf{t}\|^{2}$, without a normalizer. This would correspond to the sum of losses, and not the averaged loss. The minimizer does not depend on $N$ (but optimization might!).
- We can also add a column of 1's to design matrix, combine the bias and the weights, and conveniently write

$$
\mathbf{X}=\left[\begin{array}{cc}
1 & {\left[\mathbf{x}^{(1)}\right]^{\top}} \\
1 & {\left[\mathbf{x}^{(2)}\right]^{\top}} \\
1 & \vdots
\end{array}\right] \in \mathbb{R}^{N \times(D+1)} \quad \text { and } \mathbf{w}=\left[\begin{array}{c}
b \\
w_{1} \\
w_{2} \\
\vdots
\end{array}\right] \in \mathbb{R}^{D+1}
$$

Then, our predictions reduce to $\mathbf{y}=\mathbf{X w}$.

# Optimization 

## Solving the Minimization Problem

We defined a cost function $\mathcal{J}(\mathbf{w})$. This is what we'd like to minimize.

Recall from calculus: the minimum of a smooth function (if it exists) occurs at a critical point, i.e. point where the derivative is zero.

- multivariate generalization: set the partial derivatives $\partial \mathcal{J} / \partial w_{j}$ to zero.
- Equivalently, we can set the gradient to zero. The gradient is the vector of partial derivatives:

$$
\nabla_{\mathbf{w}} \mathcal{J}=\frac{\partial \mathcal{J}}{\partial \mathbf{w}}=\left(\begin{array}{c}
\frac{\partial \mathcal{J}}{\partial w_{1}} \\
\vdots \\
\frac{\partial \mathcal{J}}{\partial w_{D}}
\end{array}\right)
$$

Solutions may be direct or iterative

- Sometimes we can directly find provably optimal parameters (e.g. set the gradient to zero and solve in closed form). We call this a direct solution.
- Iterative solution methods repeatedly apply an update rule that gradually takes us closer to the soltuion.


## Direct Solution: Calculus

- Lets consider a cartoon visualization of $\mathcal{J}(w)$ where $w$ is single dimensional
- Left We seek $w=w^{*}$ that minimizes $\mathcal{J}(w)$
- Right The gradients of a function can tell us where the maxima and minima of functions lie
- Strategy: Write down an algebraic expression for $\nabla_{w} \mathcal{J}(w)$. Set equation to 0 . Solve for $w$




## Direct Solution: Calculus

- We seek $\mathbf{w}$ to minimize $\mathcal{J}(\mathbf{w})=\frac{1}{2}\|\mathbf{X w}-\mathbf{t}\|^{2}$
- Taking the gradient with respect to $\mathbf{w}$ (see course notes for additional details) and setting it to $\mathbf{0}$, we get:

$$
\nabla_{\mathbf{w}} \mathcal{J}(\mathbf{w})=\mathbf{X}^{\top} \mathbf{X} \mathbf{w}-\mathbf{X}^{\top} \mathbf{t}=\mathbf{0}
$$

- Optimal weights:

$$
\mathbf{w}^{*}=\left(\mathbf{X}^{\top} \mathbf{X}\right)^{-1} \mathbf{X}^{\top} \mathbf{t}
$$

- Linear regression is one of only a handful of models in this course that permit direct solution.


## Iterative solution: Gradient Descent

- Most optimization problems we cover in this course don't have a direct solution.
- Now let's see a second way to minimize the cost function which is more broadly applicable: gradient descent.
- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.



## Gradient Descent

- Observe:
- if $\partial \mathcal{J} / \partial w_{j}>0$, then increasing $w_{j}$ increases $\mathcal{J}$.
- if $\partial \mathcal{J} / \partial w_{j}<0$, then increasing $w_{j}$ decreases $\mathcal{J}$.
- The following update always decreases the cost function for small enough $\alpha$ (unless $\partial \mathcal{J} / \partial w_{j}=0$ ):

$$
w_{j} \leftarrow w_{j}-\alpha \frac{\partial \mathcal{J}}{\partial w_{j}}
$$

- $\alpha>0$ is a learning rate (or step size). The larger it is, the faster $\mathbf{w}$ changes.
- We'll see later how to tune the learning rate, but values are typically small, e.g. 0.01 or 0.0001 .
- If cost is the sum of $N$ individual losses rather than their average, smaller learning rate will be needed $\left(\alpha^{\prime}=\alpha / N\right)$.


## Gradient Descent

- This gets its name from the gradient. Recall the definition:

$$
\nabla_{\mathbf{w}} \mathcal{J}=\frac{\partial \mathcal{J}}{\partial \mathbf{w}}=\left(\begin{array}{c}
\frac{\partial \mathcal{J}}{\partial w_{1}} \\
\vdots \\
\frac{\partial \mathcal{J}}{\partial w_{D}}
\end{array}\right)
$$

- This is the direction of fastest increase in $\mathcal{J}$.
- Update rule in vector form:

$$
\mathbf{w} \leftarrow \mathbf{w}-\alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}
$$

And for linear regression we have:

$$
\mathbf{w} \leftarrow \mathbf{w}-\frac{\alpha}{N} \sum_{i=1}^{N}\left(y^{(i)}-t^{(i)}\right) \mathbf{x}^{(i)}
$$

- So gradient descent updates $\mathbf{w}$ in the direction of fastest decrease.
- Observe that once it converges, we get a critical point, i.e. $\frac{\partial \mathcal{J}}{\partial \mathbf{w}}=\mathbf{0}$.


## Gradient Descent for Linear Regression

- Even for linear regression, where there is a direct solution, we sometimes need to use GD.
- Why gradient descent, if we can find the optimum directly?
- GD can be applied to a much broader set of models
- GD can be easier to implement than direct solutions
- For regression in high-dimensional space, GD is more efficient than direct solution
- Linear regression solution: $\left(\mathbf{X}^{\top} \mathbf{X}\right)^{-1} \mathbf{X}^{\top} \mathbf{t}$
- Matrix inversion is an $\mathcal{O}\left(D^{3}\right)$ algorithm
- Each GD update costs $\mathcal{O}(N D)$
- Or less with stochastic gradient descent (SGD, covered next week)
- Huge difference if $D \gg 1$


# Feature Mappings 

## Feature Mapping (Basis Expansion)

The relation between the input and output may not be linear.


- We can still use linear regression by mapping the input features to another space using feature mapping (or basis expansion). $\boldsymbol{\psi}(\mathbf{x}): \mathbb{R}^{D} \rightarrow \mathbb{R}^{d}$ and treat the mapped feature (in $\mathbb{R}^{d}$ ) as the input of a linear regression procedure.
- Let us see how it works when $\mathbf{x} \in \mathbb{R}$ and we use a polynomial feature mapping.


## Polynomial Feature Mapping

If the relationship doesn't look linear, we can fit a polynomial.


Fit the data using a degree- $M$ polynomial function of the form:

$$
y=w_{0}+w_{1} x+w_{2} x^{2}+\ldots+w_{M} x^{M}=\sum_{i=0}^{M} w_{i} x^{i}
$$

- Here the feature mapping is $\boldsymbol{\psi}(x)=\left[1, x, x^{2}, \ldots, x^{M}\right]^{\top}$.
- We can still use linear regression to find $\mathbf{w}$ since $y=\boldsymbol{\psi}(x)^{\top} \mathbf{w}$ is linear in $w_{0}, w_{1}, \ldots$.
- In general, $\boldsymbol{\psi}$ can be any function. Another example: $\boldsymbol{\psi}(x)=[1, \sin (2 \pi x), \cos (2 \pi x), \sin (4 \pi x), \ldots]^{\top}$.


## Polynomial Feature Mapping with $M=0$


-Pattern Recognition and Machine Learning, Christopher Bishop.

## Polynomial Feature Mapping with $M=1$


-Pattern Recognition and Machine Learning, Christopher Bishop.

## Polynomial Feature Mapping with $M=3$


-Pattern Recognition and Machine Learning, Christopher Bishop.

## Polynomial Feature Mapping with $M=9$

$$
y=w_{0}+w_{1} x+w_{2} x^{2}+w_{3} x^{3}+\ldots+w_{9} x^{9}
$$


-Pattern Recognition and Machine Learning, Christopher Bishop.

## Model Complexity and Generalization

Underfitting $(\mathrm{M}=0)$ : model is too simple - does not fit the data. Overfitting ( $M=9$ ): model is too complex - fits perfectly.




Good model $(\mathrm{M}=3)$ : Achieves small test error (generalizes well).


## Model Complexity and Generalization

|  | $M=0$ | $M=1$ | $M=3$ | $M=9$ |
| ---: | ---: | ---: | ---: | ---: |
| $w_{0}^{\star}$ | 0.19 | 0.82 | 0.31 | 0.35 |
| $w_{1}^{\star}$ |  | -1.27 | 7.99 | 232.37 |
| $w_{2}^{\star}$ |  |  | -25.43 | -5321.83 |
| $w_{3}^{\star}$ |  |  | 17.37 | 48568.31 |
| $w_{4}^{\star}$ |  |  |  | -231639.30 |
| $w_{5}^{\star}$ |  |  |  | 640042.26 |
| $w_{6}^{\star}$ |  |  |  | -1061800.52 |
| $w_{7}^{\star}$ |  |  |  | 1042400.18 |
| $w_{8}^{\star}$ |  |  |  | -557682.99 |
| $w_{9}^{\star}$ |  |  |  | 125201.43 |



- As $M$ increases, the magnitude of coefficients gets larger.
- For $M=9$, the coefficients have become finely tuned to the data.
- Between data points, the function exhibits large oscillations.


# Regularization 

## Regularization

- The degree $M$ of the polynomial controls the model's complexity.
- The value of $M$ is a hyperparameter for polynomial expansion, just like $k$ in KNN. We can tune it using a validation set.
- Restricting the number of parameters / basis functions $(M)$ is a crude approach to controlling the model complexity.
- Another approach: keep the model large, but regularize it
- Regularizer: a function that quantifies how much we prefer one hypothesis vs. another


## $L^{2}\left(\right.$ or $\left.\ell_{2}\right)$ Regularization

- We can encourage the weights to be small by choosing as our regularizer the $L^{2}$ penalty.

$$
\mathcal{R}(\mathbf{w})=\frac{1}{2}\|\mathbf{w}\|_{2}^{2}=\frac{1}{2} \sum_{j} w_{j}^{2}
$$

- Note: To be precise, the $L^{2}$ norm $\|\mathbf{w}\|_{2}$ is Euclidean distance, so we're regularizing the squared $L^{2}$ norm.
- The regularized cost function makes a tradeoff between fit to the data and the norm of the weights.

$$
\mathcal{J}_{\mathrm{reg}}(\mathbf{w})=\mathcal{J}(\mathbf{w})+\lambda \mathcal{R}(\mathbf{w})=\mathcal{J}(\mathbf{w})+\frac{\lambda}{2} \sum_{j} w_{j}^{2}
$$

- If you fit training data poorly, $\mathcal{J}$ is large. If the weights are large in magnitude, $\mathcal{R}$ is large.
- Large $\lambda$ penalizes weight values more.
- $\lambda$ is a hyperparameter we can tune with a validation set.


## $L^{2}$ (or $\ell_{2}$ ) Regularization

- The geometric picture:



## $L^{2}$ Regularized Least Squares: Ridge regression

For the least squares problem, we have $\mathcal{J}(\mathbf{w})=\frac{1}{2 N}\|\mathbf{X w}-\mathbf{t}\|^{2}$.

- When $\lambda>0$ (with regularization), regularized cost gives

$$
\begin{aligned}
\mathbf{w}_{\lambda}^{\text {Ridge }}=\underset{\mathbf{w}}{\operatorname{argmin}} \mathcal{J}_{\text {reg }}(\mathbf{w}) & =\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2 N}\|\mathbf{X} \mathbf{w}-\mathbf{t}\|_{2}^{2}+\frac{\lambda}{2}\|\mathbf{w}\|_{2}^{2} \\
& =\left(\mathbf{X}^{\top} \mathbf{X}+\lambda N \mathbf{I}\right)^{-1} \mathbf{X}^{\top} \mathbf{t}
\end{aligned}
$$

- The case $\lambda=0$ (no regularization) reduces to least squares solution!
- Note that it is also common to formulate this problem as $\operatorname{argmin}_{\mathbf{w}} \frac{1}{2}\|\mathbf{X w}-\mathbf{t}\|_{2}^{2}+\frac{\lambda}{2}\|\mathbf{w}\|_{2}^{2}$ in which case the solution is $\mathbf{w}_{\lambda}^{\text {Ridge }}=\left(\mathbf{X}^{\top} \mathbf{X}+\lambda \mathbf{I}\right)^{-1} \mathbf{X}^{\top} \mathbf{t}$.


## Gradient Descent under the $L^{2}$ Regularization

- Gradient descent update to minimize $\mathcal{J}$ :

$$
\mathbf{w} \leftarrow \mathbf{w}-\alpha \frac{\partial}{\partial \mathbf{w}} \mathcal{J}
$$

- The gradient descent update to minimize the $L^{2}$ regularized cost $\mathcal{J}+\lambda \mathcal{R}$ results in weight decay:

$$
\begin{aligned}
\mathbf{w} & \leftarrow \mathbf{w}-\alpha \frac{\partial}{\partial \mathbf{w}}(\mathcal{J}+\lambda \mathcal{R}) \\
& =\mathbf{w}-\alpha\left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}}+\lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}}\right) \\
& =\mathbf{w}-\alpha\left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}}+\lambda \mathbf{w}\right) \\
& =(1-\alpha \lambda) \mathbf{w}-\alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}
\end{aligned}
$$

## Conclusion so far

Linear regression exemplifies recurring themes of this course:

- choose a model and a loss function
- formulate an optimization problem
- solve the minimization problem using one of two strategies
- direct solution (set derivatives to zero)
- gradient descent
- vectorize the algorithm, i.e. represent in terms of linear algebra
- make a linear model more powerful using features
- improve the generalization by adding a regularizer

