CSC 311: Introduction to Machine Learning

Lecture 2 - Linear Methods for Regression, Optimization

Roger Grosse Chris Maddison Juhan Bae Silviu Pitis

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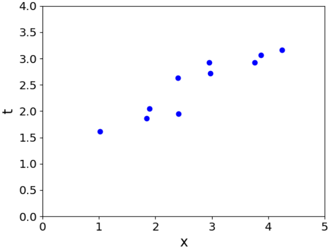
Announcements

- Homework 1 is posted! Deadline Sept 30, 23:59.
- Instructor hours are announced on the course website. (TA OH TBA)
- No ProctorU!

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 $\mathcal{D} = \{(\mathbf{x}^{(i)}, t^{(i)}) \text{ for } i = 1, 2, ..., N\}$.

Linear Regression - Model

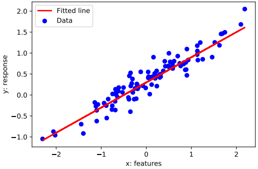
- Model: In linear regression, we use a *linear* function of the features $\mathbf{x} = (x_1, \ldots, x_D) \in \mathbb{R}^D$ to make predictions y of the target value $t \in \mathbb{R}$:

$$y = f(\mathbf{x}) = \sum_j w_j x_j + b$$

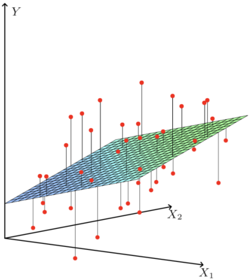
  - y is the prediction
  - $\mathbf{w}$ is the weights
  - b is the bias (or intercept)

- $\mathbf{w}$ 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:
  $y = wx + b$ where $w, x, b \in \mathbb{R}$.
- y is linear in x.



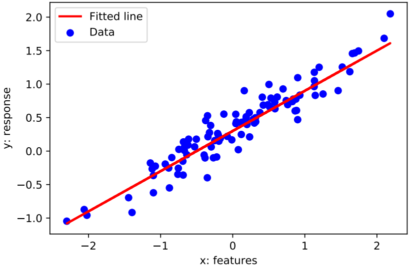
- If we have D features:
  $y = \mathbf{w}^\top \mathbf{x} + b$ where $\mathbf{w}, \mathbf{x} \in \mathbb{R}^D$,
  $b \in \mathbb{R}$
- y is linear in $\mathbf{x}$.

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

Linear Regression

We have a dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, t^{(i)})$ for $i = 1, 2, ..., N\}$ where,

- $\mathbf{x}^{(i)} = (x_1^{(i)}, x_2^{(i)}, ..., x_D^{(i)})^\top \in \mathbb{R}^D$ are the inputs (e.g. age, height)
- $t^{(i)} \in \mathbb{R}$ is the target or response (e.g. income)
- predict $t^{(i)}$ with a linear function of $\mathbf{x}^{(i)}$:



- $t^{(i)} \approx y^{(i)} = \mathbf{w}^\top \mathbf{x}^{(i)} + b$
- Different $(\mathbf{w}, b)$ define different lines.
- We want the "best" line $(\mathbf{w}, b)$.
- How to quantify "best"?

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:

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

- $y - t$ 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

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

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

Vectorization

- Notation-wise, $\frac{1}{2N}\sum_{i=1}^{N}\left(y^{(i)}-t^{(i)}\right)^2$ gets messy if we expand $y^{(i)}$:

$$\frac{1}{2N}\sum_{i=1}^{N}\left(\sum_{j=1}^{D}\left(w_j x_j^{(i)}+b\right)-t^{(i)}\right)^2$$

- The code equivalent is to compute the prediction using a for loop:

```
y = b
for j in range(M):
    y += w[j] * x[j]
```

- 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.

$$\mathbf{w}=(w_1,\ldots,w_D)^\top \qquad \mathbf{x}=(x_1,\ldots,x_D)^\top$$

$$y=\mathbf{w}^\top\mathbf{x}+b$$

- This is simpler and executes much faster:

```
y = np.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
all training examples

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \end{pmatrix} = \begin{pmatrix} 8 & 0 & 3 & 0 \\ 6 & -1 & 5 & 3 \\ 2 & 5 & -2 & 8 \end{pmatrix}$$

one training
example (vector)

- Computing the predictions for the whole dataset:

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

Vectorization

- Computing the squared error cost across the whole dataset:

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

- 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

$$\mathbf{X} = \begin{bmatrix} 1 & [\mathbf{x}^{(1)}]^\top \\ 1 & [\mathbf{x}^{(2)}]^\top \\ 1 & \vdots \end{bmatrix} \in \mathbb{R}^{N \times (D+1)} \text{ and } \mathbf{w} = \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \end{bmatrix} \in \mathbb{R}^{D+1}$$

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

Solving the Minimization Problem

We defined a cost function. This is what we'd like to minimize.

Two commonly applied mathematical approaches:

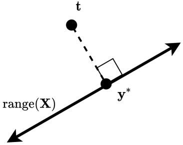
- Algebraic, e.g., using inequalities:
  - to show z^* minimizes $f(z)$, show that $\forall z, f(z) \geq f(z^*)$
  - to show that $a = b$, show that $a \geq b$ and $b \geq a$
- Calculus: minimum of a smooth function (if it exists) occurs at a critical point, i.e. point where the derivative is zero.
  - multivariate generalization: set the partial derivatives to zero (or equivalently the gradient).

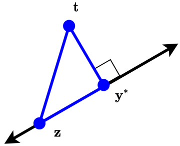
Solutions may be direct or iterative

- 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.
- We may also use optimization techniques that iteratively get us closer to the solution. We will get back to this soon.

Direct Solution I: Linear Algebra

- We seek $\mathbf{w}$ to minimize $\|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$, or equivalently $\|\mathbf{X}\mathbf{w} - \mathbf{t}\|$
- $\text{range}(\mathbf{X}) = \{\mathbf{X}\mathbf{w} \mid \mathbf{w} \in \mathbb{R}^D\}$ is a D-dimensional subspace of $\mathbb{R}^N$.
- Recall that the closest point $\mathbf{y}^* = \mathbf{X}\mathbf{w}^*$ in subspace $\text{range}(\mathbf{X})$ of $\mathbb{R}^N$ to arbitrary point $\mathbf{t} \in \mathbb{R}^N$ is found by orthogonal projection.





- We have $(\mathbf{y}^* - \mathbf{t}) \perp \mathbf{X}\mathbf{w}, \ \forall \mathbf{w} \in \mathbb{R}^D$
- Why is $\mathbf{y}^*$ the closest point to $\mathbf{t}$?
  - Consider any $\mathbf{z} = \mathbf{X}\mathbf{w}$
  - By Pythagorean theorem and the trivial inequality ($x^2 \geq 0$):

$$\begin{aligned} \|\mathbf{z} - \mathbf{t}\|^2 &= \|\mathbf{y}^* - \mathbf{t}\|^2 + \|\mathbf{y}^* - \mathbf{z}\|^2 \\ &\geq \|\mathbf{y}^* - \mathbf{t}\|^2 \end{aligned}$$

Direct Solution I: Linear Algebra

- From the previous slide, we have $(\mathbf{y}^* - \mathbf{t}) \perp \mathbf{X}\mathbf{w}, \ \forall \mathbf{w} \in \mathbb{R}^D$
- Equivalently, the columns of the design matrix $\mathbf{X}$ are all orthogonal to $(\mathbf{y}^* - \mathbf{t})$, and we have that:

$$\begin{aligned}
\mathbf{X}^\top(\mathbf{y}^* - \mathbf{t}) &= \mathbf{0} \\
\mathbf{X}^\top\mathbf{X}\mathbf{w}^* - \mathbf{X}^\top\mathbf{t} &= \mathbf{0} \\
\mathbf{X}^\top\mathbf{X}\mathbf{w}^* &= \mathbf{X}^\top\mathbf{t} \\
\mathbf{w}^* &= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{t}
\end{aligned}$$

- While this solution is clean and the derivation easy to remember, like many algebraic solutions, it is somewhat ad hoc.
- On the hand, the tools of calculus are broadly applicable to differentiable loss functions...

Direct Solution II: Calculus

- Partial derivative: derivative of a multivariate function with respect to one of its arguments.

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$

- To compute, take the single variable derivative, pretending the other arguments are constant.
- Example: partial derivatives of the prediction y

$$\begin{aligned} \frac{\partial y}{\partial w_j} &= \frac{\partial}{\partial w_j} \left[\sum_{j'} w_{j'} x_{j'} + b \right] \\ &= x_j \end{aligned} \qquad \begin{aligned} \frac{\partial y}{\partial b} &= \frac{\partial}{\partial b} \left[\sum_{j'} w_{j'} x_{j'} + b \right] \\ &= 1 \end{aligned}$$

Direct Solution II: Calculus

- For loss derivatives, apply the chain rule:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\frac{\partial y}{\partial w_j} \\ &= \frac{\mathrm{d}}{\mathrm{d}y}\left[\frac{1}{2}(y-t)^2\right]\cdot x_j \\ &= (y-t)x_j\end{aligned}$$

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial b} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\frac{\partial y}{\partial b} \\ &= y-t\end{aligned}$$

- For cost derivatives, use linearity and average over data points:

$$\frac{\partial \mathcal{J}}{\partial w_j} = \frac{1}{N}\sum_{i=1}^{N}(y^{(i)}-t^{(i)})\,x_j^{(i)} \qquad \frac{\partial \mathcal{J}}{\partial b} = \frac{1}{N}\sum_{i=1}^{N} y^{(i)}-t^{(i)}$$

- Minimum must occur at a point where partial derivatives are zero.

$$\frac{\partial \mathcal{J}}{\partial w_j} = 0 \quad (\forall j), \qquad \frac{\partial \mathcal{J}}{\partial b} = 0.$$

(if $\partial \mathcal{J}/\partial w_j \neq 0$, you could reduce the cost by changing w_j)

Direct Solution II: Calculus

- The derivation on the previous slide gives a system of linear equations, which we can solve efficiently.
- As is often the case for models and code, however, the solution is easier to characterize if we vectorize our calculus.
- We call the vector of partial derivatives the gradient
- Thus, the "gradient of $f : \mathbb{R}^D \to \mathbb{R}$", denoted $\nabla f(\mathbf{w})$, is:

$$\left(\frac{\partial}{\partial w_1} f(\mathbf{w}), \dots, \frac{\partial}{\partial w_D} f(\mathbf{w}) \right)^\top$$

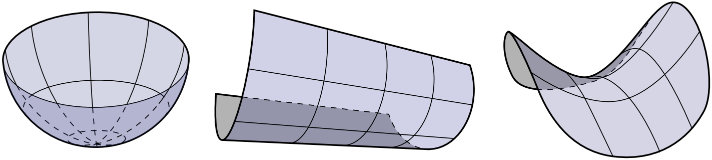
- The gradient points in the direction of the greatest rate of increase.
- Analogue of second derivative (the "Hessian" matrix): $\nabla^2 f(\mathbf{w}) \in \mathbb{R}^{D \times D}$ is a matrix with $[\nabla^2 f(\mathbf{w})]_{ij} = \frac{\partial^2}{\partial w_i \partial w_j} f(\mathbf{w})$.

Aside: The Hessian Matrix

- Analogue of second derivative (the Hessian): $\nabla^2 f(\mathbf{w}) \in \mathbb{R}^{D \times D}$ is a matrix with $[\nabla^2 f(\mathbf{w})]_{ij} = \frac{\partial^2}{\partial w_i \partial w_j} f(\mathbf{w})$.
  - Recall from multivariable calculus that for continuously differentiable f, $\frac{\partial^2}{\partial w_i \partial w_j} f = \frac{\partial^2}{\partial w_j \partial w_i} f$, so the Hessian is symmetric.
- The second derivative test in single variable calculus: a critical point is a local minimum if the second derivative is positive.
- The multivariate analogue involves the eigenvalues of the Hessian.
  - Recall from linear algebra that the eigenvalues of a symmetric matrix (and therefore the Hessian) are real-valued.
  - If all of the eigenvalues are positive, we say the Hessian is positive definite.
  - A critical point ($\nabla f(\mathbf{w}) = \mathbf{0}$) of a continuously differentiable function f is a local minimum if the Hessian is positive definite.

Aside: The Hessian Matrix

- Visualization:[1]



$x^2 + y^2$ (definite) $\qquad$ x^2 (semidefinite) $\qquad$ $x^2 - y^2$ (indefinite)

[1] Image source: mkwiki.org

Direct Solution II: Calculus

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

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

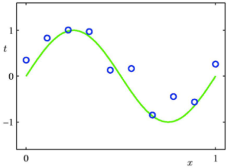
- We get the same optimal weights as before:

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

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

Feature Mapping (Basis Expansion)

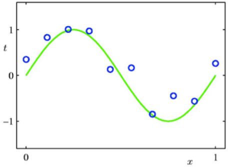
The relation between the input and output may not be linear.



- We can still use linear regression by mapping the input features to another space using feature mapping (or basis expansion). $\boldsymbol{\psi}(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}^d$ 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.



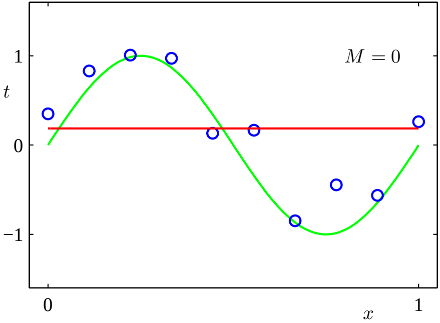
Fit the data using a degree-M polynomial function of the form:

$$y = w_0 + w_1 x + w_2 x^2 + ... + w_M x^M = \sum_{i=0}^{M} w_i x^i$$

- Here the feature mapping is $\boldsymbol{\psi}(x) = [1, x, x^2, ..., x^M]^\top$.
- We can still use linear regression to find $\mathbf{w}$ since $y = \boldsymbol{\psi}(x)^\top \mathbf{w}$ is linear in $w_0, w_1, ...$.
- In general, $\boldsymbol{\psi}$ can be any function. Another example: $\boldsymbol{\psi}(x) = [1, \sin(2\pi x), \cos(2\pi x), \sin(4\pi x), ...]^\top$.

Polynomial Feature Mapping with $M = 0$

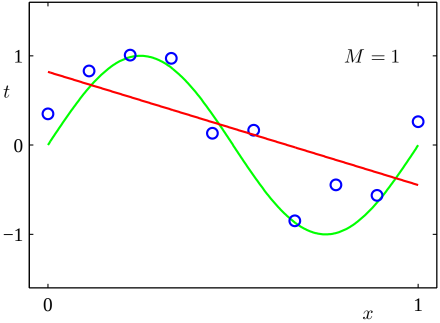
$$y = w_0$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Polynomial Feature Mapping with $M = 1$

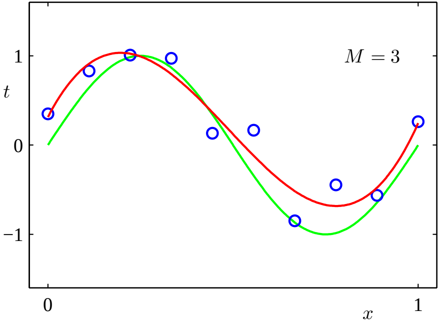
$$y = w_0 + w_1 x$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Polynomial Feature Mapping with $M = 3$

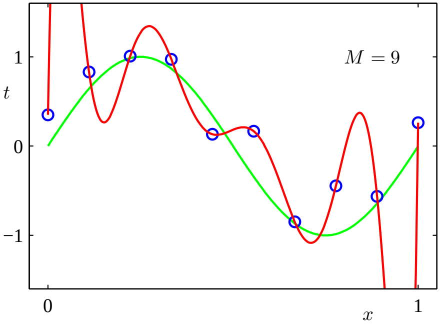
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Polynomial Feature Mapping with $M = 9$

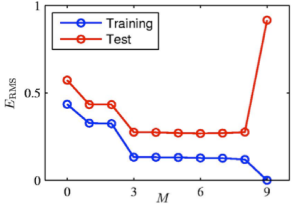
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$

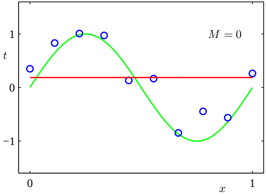


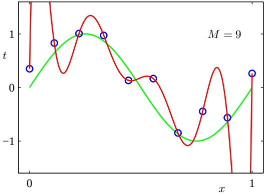
-Pattern Recognition and Machine Learning, Christopher Bishop.

Model Complexity and Generalization

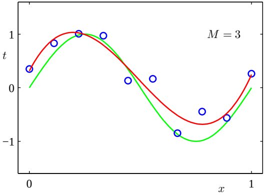
Underfitting (M=0): model is too simple — does not fit the data.
Overfitting (M=9): model is too complex — fits perfectly.





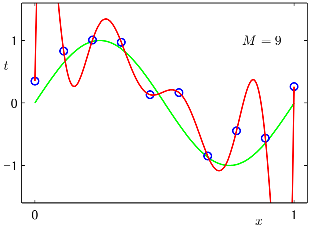


Good model (M=3): Achieves small test error (generalizes well).



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

- 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 (or ℓ_2) Regularization

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

$$\mathcal{R}(\mathbf{w}) = \tfrac{1}{2}\|\mathbf{w}\|_2^2 = \frac{1}{2}\sum_j w_j^2.$$

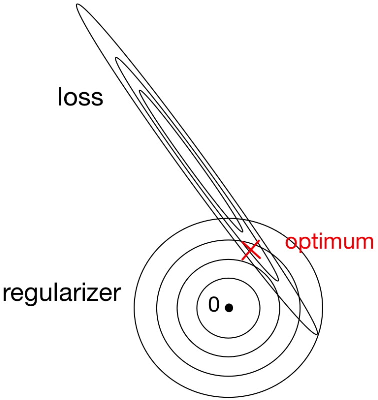
  - Note: To be precise, the L^2 norm is Euclidean distance, so we're regularizing the *squared* L^2 norm.
- The regularized cost function makes a tradeoff between fit to the data and the norm of the weights.

$$\mathcal{J}_{\text{reg}}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \lambda\mathcal{R}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \frac{\lambda}{2}\sum_j w_j^2$$

- If you fit training data poorly, $\mathcal{J}$ is large. If your optimal weights have high values, $\mathcal{R}$ is large.
- Large λ penalizes weight values more.
- Like M, λ is a hyperparameter we can tune with a validation set.

L^2 (or ℓ_2) Regularization

- The geometric picture:



L^2 Regularized Least Squares: Ridge regression

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

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

$$\begin{aligned}\mathbf{w}_\lambda^{\text{Ridge}} = \underset{\mathbf{w}}{\operatorname{argmin}}\, \mathcal{J}_{\text{reg}}(\mathbf{w}) =& \underset{\mathbf{w}}{\operatorname{argmin}}\, \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2 \\ =& (\mathbf{X}^\top\mathbf{X} + \lambda N\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{t}\end{aligned}$$

- The case $\lambda = 0$ (no regularization) reduces to least squares solution!
- Note that it is also common to formulate this problem as $\operatorname{argmin}_{\mathbf{w}} \frac{1}{2}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$ in which case the solution is $\mathbf{w}_\lambda^{\text{Ridge}} = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{t}$.

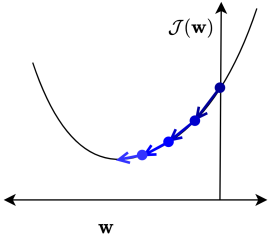
Conclusion so far

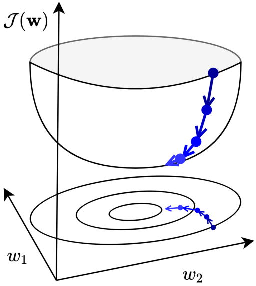
Linear regression exemplifies recurring themes of this course:

- 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 (next topic)
- 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

Gradient Descent

- Now let's see a second way to minimize the cost function which is more broadly applicable: gradient descent.
- Many times, we do not have a direct solution: Taking derivatives of $\mathcal{J}$ w.r.t $\mathbf{w}$ and setting them to 0 doesn't have an explicit solution.
- 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 α (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 ($\alpha' = \alpha/N$).

Gradient Descent

- This gets its name from the gradient:

$$\nabla_{\mathbf{w}} \mathcal{J} = \frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial w_D} \end{pmatrix}$$

  - 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:

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

- 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

- The squared error loss of linear regression is a convex function.
- 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: $(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$
    - Matrix inversion is an $\mathcal{O}(D^3)$ algorithm
    - Each GD update costs $\mathcal{O}(ND)$
    - Or less with stochastic GD (SGD, in a few slides)
    - Huge difference if $D \gg 1$

Gradient Descent under the L^2 Regularization

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

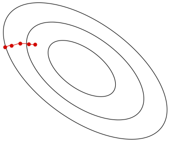
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} \mathcal{J}$$

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

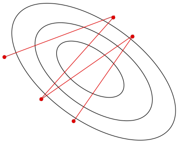
$$\begin{aligned}
\mathbf{w} &\leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} (\mathcal{J} + \lambda \mathcal{R}) \\
&= \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right) \\
&= \mathbf{w} -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

Learning Rate (Step Size)

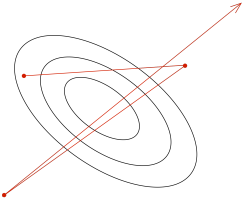
- In gradient descent, the learning rate α is a hyperparameter we need to tune. Here are some things that can go wrong:



α too small: slow progress



α too large: oscillations

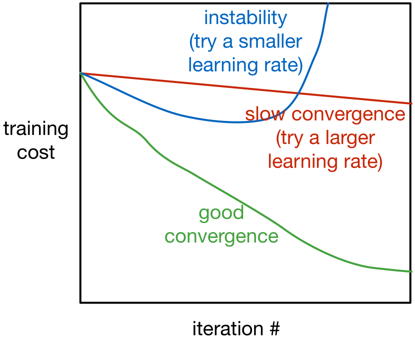


α much too large: instability

- 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.



- Warning: in general, 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:

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

  ($\boldsymbol{\theta}$ denotes the parameters; e.g., in linear regression, $\boldsymbol{\theta} = (\mathbf{w}, b)$)
- 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 $N \gg 1$ (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,

$$\begin{aligned} 1- \qquad & \text{Choose } i \text{ uniformly at random,} \\ 2- \qquad & \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} \end{aligned}$$

- Cost of each SGD update is independent of N!
- SGD can make significant progress before even seeing all the data!
- Mathematical justification: if you sample a training example uniformly at random, the stochastic gradient is an unbiased estimate of the batch gradient:

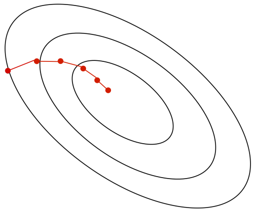
$$\mathbb{E}\left[\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}\right] = \frac{1}{N}\sum_{i=1}^{N} \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}.$$

Stochastic Gradient Descent

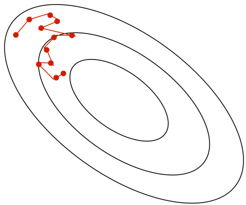
- Problems with using single training example to estimate gradient:
  - Variance in the estimate may be high
  - We can't exploit efficient vectorized operations
- Compromise approach:
  - compute the gradients on a randomly chosen medium-sized set of training examples $\mathcal{M} \subset \{1, \ldots, N\}$, called a mini-batch.
- Stochastic gradients computed on larger mini-batches have smaller variance.
- The mini-batch size $|\mathcal{M}|$ is a hyperparameter that needs to be set.
  - Too large: requires more compute; e.g., it takes more memory to store the activations, and longer to compute each gradient update
  - Too small: can't exploit vectorization, has high variance
  - A reasonable value might be $|\mathcal{M}| = 100$.

Stochastic Gradient Descent

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



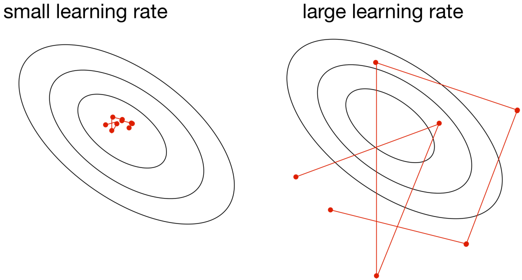
batch gradient descent



stochastic gradient descent

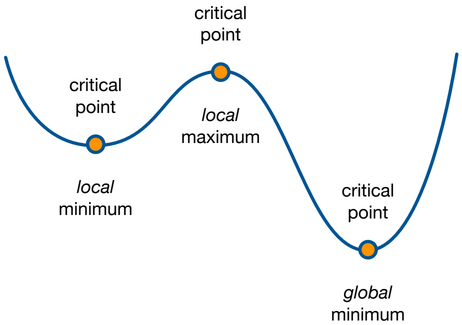
SGD Learning Rate

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



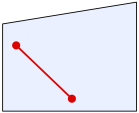
- Typical strategy:
  - Use a large learning rate early in training so you can get close to the optimum
  - Gradually decay the learning rate to reduce the fluctuations

When are critical points optimal?



- Gradient descent finds a critical point, but it may be a local optima.
- Convexity is a property that guarantees that all critical points are global minima.

Convex Sets



- A set $\mathcal{S}$ is convex if any line segment connecting points in $\mathcal{S}$ lies entirely within $\mathcal{S}$. Mathematically,

$$\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{S} \implies \lambda \mathbf{x}_1 + (1-\lambda)\mathbf{x}_2 \in \mathcal{S} \quad \text{for } 0 \leq \lambda \leq 1.$$

- A simple inductive argument shows that for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathcal{S}$, weighted averages, or convex combinations, lie within the set:

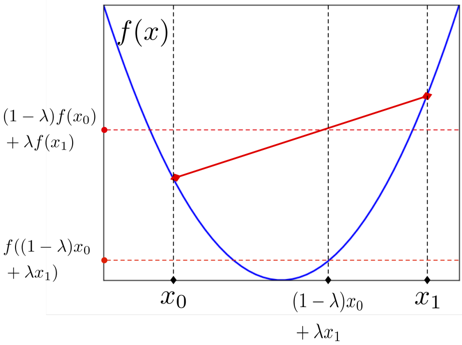
$$\lambda_1 \mathbf{x}_1 + \cdots + \lambda_N \mathbf{x}_N \in \mathcal{S} \quad \text{for } \lambda_i > 0, \; \lambda_1 + \cdots \lambda_N = 1.$$

Convex Functions

- A function f is convex if for any $\mathbf{x}_0, \mathbf{x}_1$ in the domain of f,

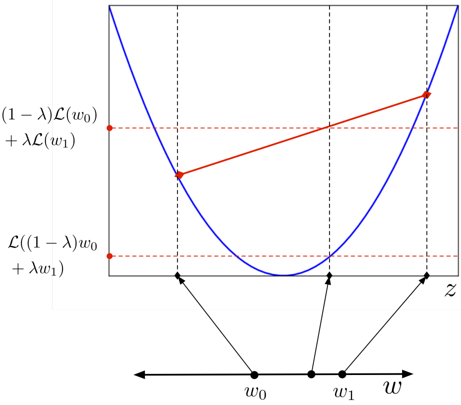
$$f((1-\lambda)\mathbf{x}_0 + \lambda\mathbf{x}_1) \leq (1-\lambda)f(\mathbf{x}_0) + \lambda f(\mathbf{x}_1)$$

- Equivalently, the set of points lying above the graph of f is convex.
- Intuitively: the function is bowl-shaped.



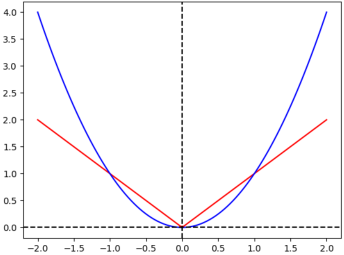
Convex Functions

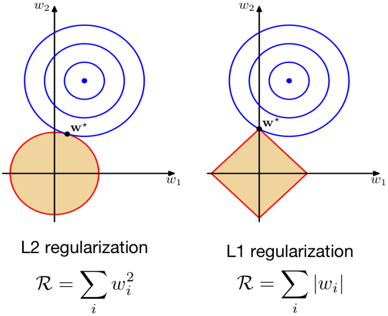
- We just saw that the least-squares loss $\frac{1}{2}(y-t)^2$ is convex as a function of y
- For a linear model, $z = \mathbf{w}^\top \mathbf{x} + b$ is a linear function of $\mathbf{w}$ and b. If the loss function is convex as a function of z, then it is convex as a function of $\mathbf{w}$ and b.



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.

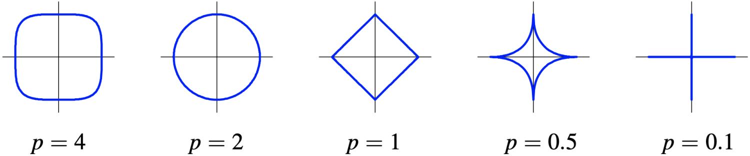




— Bishop, *Pattern Recognition and Machine Learning*

Linear Regression with L^p Regularization

Which sets are convex?



Solution of linear regression with L^p regularization:

- $p = 2$: Has a closed form solution.
- $p \geq 1, p \neq 2$:
  - The objective is convex.
  - The true solution can be found using gradient descent.
- $p < 1$:
  - The objective is non-convex.
  - Can only find approximate solution (e.g. the best in its neighborhood) using gradient descent.

Conclusion

- In this lecture, we looked at linear regression, which exemplifies a modular approach that will be used throughout this course:
  - choose a model describing the relationships between variables of interest (**linear**)
  - define a loss function quantifying how bad the fit to the data is **(squared error)**
  - choose a regularizer to control the model complexity/overfitting (L^2, L^p **regularization**)
  - fit/optimize the model (**gradient descent, stochastic gradient descent, convexity**)
- By mixing and matching these modular components, we can obtain new ML methods.
- Next lecture: apply this framework to classification