

Introduction to Machine Learning

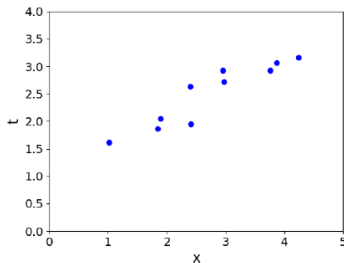
Linear Regression & Optimization

Ashley Gao

William & Mary

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Supervised Learning Setup



- In supervised learning:
 - There is input $x \in \mathcal{X}$, 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 $t \approx y = f(x)$ based on the dataset $\mathcal{D} = \{(x^{(i)}, t^{(i)})\}$ for $i = 1, 2, \dots, N$.

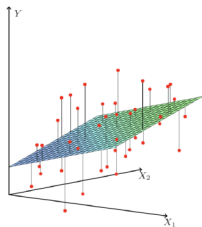
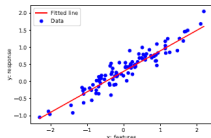
Linear Regression - Model

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

$$y = f(x) = \sum_j w_j x_j + b \quad (1)$$

- y is the prediction
- w is the weights
- b is the bias (or intercept)
- 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

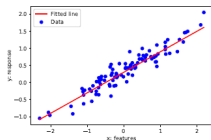


- If we have only 1 feature:
 $y = wx + b$ where $w, x, b \in \mathbb{R}$
- y is linear in x
- If we have only D feature:
 $y = \mathbf{w}^\top \mathbf{x} + b$ where $\mathbf{w}, \mathbf{x} \in \mathbb{R}^D$
and $b \in \mathbb{R}$
- y is linear in x

- Relation between the prediction y and inputs x is linear in both cases.

Linear Regression

- We have a dataset $\mathcal{D} = \{(x^{(i)}, t^{(i)})\}$ for $i = 1, 2, \dots, N$, where
 - $x^{(i)} = (x_1^{(i)}, x_2^{(i)}, \dots, x_D^{(i)})^\top \in \mathbb{R}^D$ are the inputs (i.e. age, height)
 - $t^{(i)} \in \mathbb{R}$ is the target or response (i.e. income)
 - Predict $t^{(i)}$ with a linear function of $x^{(i)}$



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

- Relation between the prediction y and inputs 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:

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

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

$$\mathcal{J}(\mathbf{w}, b) = \frac{1}{2N} \sum_{i=1}^N (y^{(i)} - t^{(i)})^2 = \frac{1}{2N} \sum_{i=1}^N (\mathbf{w}^\top \mathbf{x}^{(i)} + b - t^{(i)})^2 \quad (3)$$

- Terminology varies. Some call “cost” empirical or average loss.

Vectorization

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

$$\frac{1}{2N} \sum_{i=1}^N \left(\sum_{j=1}^D (w_j x_j^{(i)} + b) - t^{(i)} \right)^2 \quad (4)$$

- 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.

$$\mathbf{w} = (w_1, \dots, w_D)^\top; \mathbf{x} = (x_1, \dots, x_D); y = \mathbf{w}^\top \mathbf{x} + b \quad (5)$$

- This is simpler and executes much faster:

$$y = np.dot(\mathbf{w}, \mathbf{x}) + b \quad (6)$$

Vectorization

- Why vectorize?
 - The equations, and the code, will be simpler and more readable. Gets rid of dummy variables and 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 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 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:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b\mathbf{1}; \mathcal{J} = \frac{1}{2N} ||\mathbf{y} - \mathbf{t}||^2 \quad (7)$$

- Sometimes we 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

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

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

Vectorization

- We have defined a cost function. This is what we'd like to minimize.
- Two commonly applied mathematical approaches:
 - Algebraic, e.g., using inequalities:
 - To show that z^* minimizes $f(z)$, show that $\forall z, f(z) \geq f(z^*)$
 - 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: Calculus

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

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \lim_{h \rightarrow 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h} \quad (8)$$

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

$$\frac{\partial y}{\partial w_j} = \frac{\partial}{\partial w_j} \left(\sum_{j'} w_{j'} x_{j'} + b \right) = x_j \quad (9)$$

$$\frac{\partial y}{\partial b} = \frac{\partial}{\partial b} \left(\sum_{j'} w_{j'} x_{j'} + b \right) = 1 \quad (10)$$

Direct Solution: Calculus

- For loss derivatives, apply the chain rule:

$$\frac{\partial(L)}{\partial w_j} = \frac{d(L)}{dy} \frac{\partial(y)}{\partial w_j} = \frac{d}{dy} \left(\frac{1}{2} (y - t)^2 \right) x_j = (y - t) x_j \quad (11)$$

$$\frac{\partial(L)}{\partial b} = \frac{d(L)}{dy} \frac{\partial(y)}{\partial b} = y - t \quad (12)$$

- For cost derivatives, use linearity and average over data points.
- Minimum must occur at a point where partial derivatives are zero.

$$\frac{\partial(J)}{\partial w_j} = \frac{1}{N} \sum_{i=1}^N (y^{(i)} - t^{(i)}) x_j^{(i)} = 0 \quad (13)$$

$$\frac{\partial(J)}{\partial b} = \frac{1}{N} \sum_{i=1}^N y^{(i)} - t^{(i)} = 0 \quad (14)$$

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

Direct Solution: Calculus

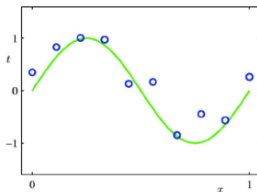
- The derivation on the previous slide gives a system of linear equations, which we can solve efficiently.
- As is often the case for models and code, however, the solution is easier to characterize if we vectorize our calculus.
- We call the vector of partial derivatives the gradient
- Thus, the gradient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

$$\left(\frac{\partial}{\partial w_1} f(\mathbf{w}), \dots, \frac{\partial}{\partial w_D} f(\mathbf{w}) \right)^\top \quad (15)$$

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

Feature Mapping (Basic Expansion)

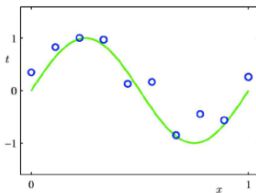
- The relation between the input and output may not be linear.



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

Feature Mapping (Basic Expansion)

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



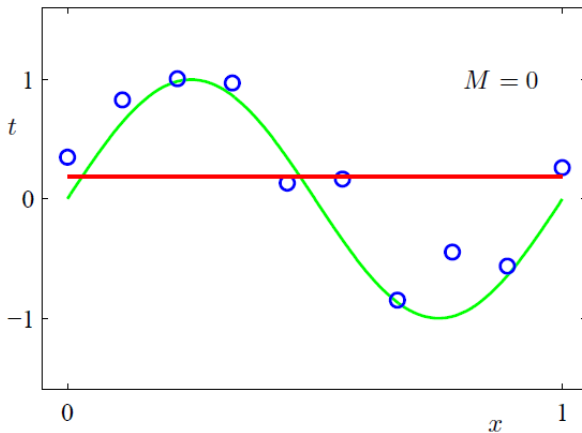
- Fit the data using a degree- M polynomial function of the form:

$$y = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{i=0}^M w_ix^i \quad (16)$$

- Here the feature mapping is $\psi(x) = [1, x, x^2, \dots, x^M]^\top$
- We can still use linear regression to find \mathbf{w} since $y = \psi(x)^\top$ is linear in w_0, w_1, \dots , because the coefficients are still **linear**!

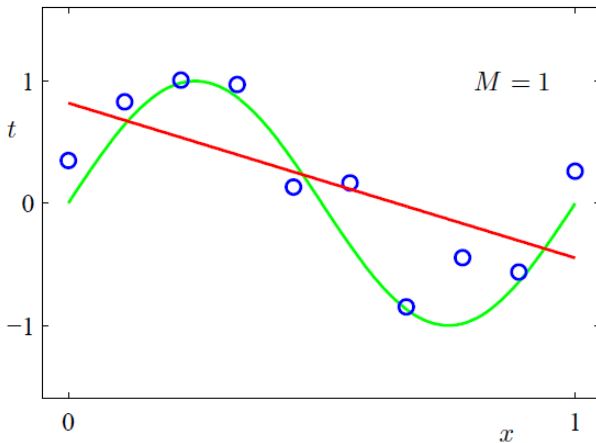
Polynomial Feature Mapping with $M = 0$

$$y = w_0$$



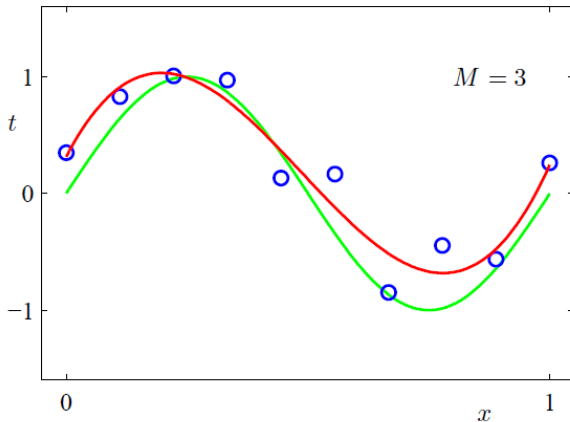
Polynomial Feature Mapping with $M = 1$

$$y = w_0 + w_1 x$$



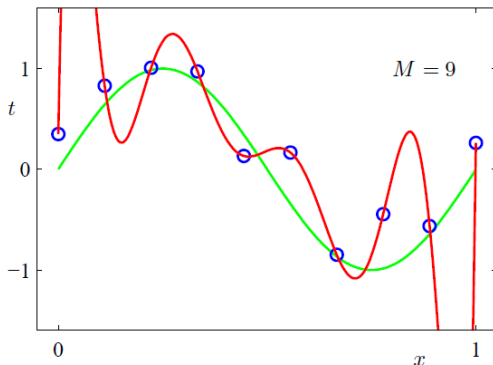
Polynomial Feature Mapping with $M = 3$

$$y = w_0 + w_1x + w_2x^2 + w_3x^3$$



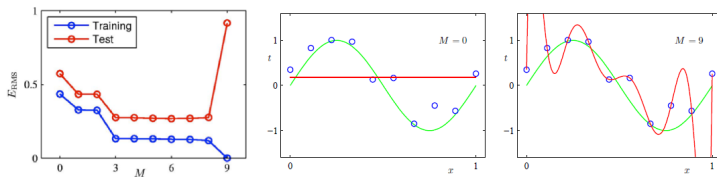
Polynomial Feature Mapping with $M = 9$

$$y = w_0 + w_1x + w_2x^2 + w_3x^3 + \dots + w_9x^9$$

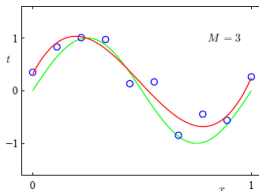


Model Complexity and Generalization

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

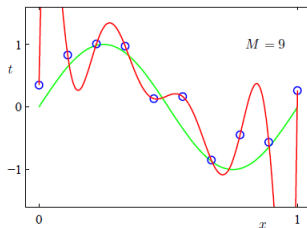


- Good model ($M=3$): Achieves small test error (generalizes well).



Model Complexity and Generalization

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
w_8^*				-557682.99
w_9^*				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 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.

$$\mathcal{R}(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|_2^2 = \frac{1}{2} \sum_j w_j^2 \quad (17)$$

- 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.

$$\mathcal{J}_{reg}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \lambda \mathcal{R}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \frac{\lambda}{2} \sum_j w_j^2 \quad (18)$$

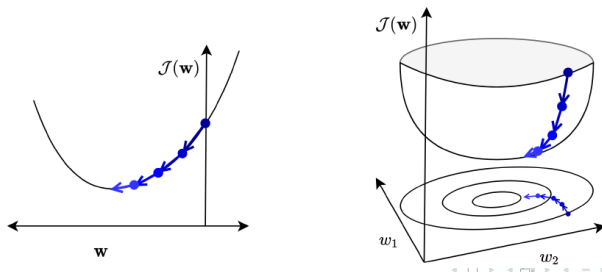
- If you fit training data poorly, \mathcal{J} is large. If your optimal weights have high values, \mathcal{R} is large. Large λ penalizes weight values more.
- Like M , λ is a hyperparameter we can tune with a validation set.

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 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 the steepest descent.



Gradient Descent

- Observe:
 - if $\frac{\partial \mathcal{J}}{\partial w_j} > 0$, then increasing w_j increases \mathcal{J}
 - if $\frac{\partial \mathcal{J}}{\partial w_j} < 0$, then increasing w_j decreases \mathcal{J}
- The following update always decreases the cost function for small enough α unless $\frac{\partial \mathcal{J}}{\partial w_j} = 0$:

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j} \quad (19)$$

- $\alpha > 0$ is a learning rate (or step size). The larger it is, the faster w changes.
 - We'll see later how to tune the learning rate, but values are typically small, e.g. 0.01 or 0.0001.

Gradient Descent

- This gets its name from the gradient:

$$\nabla_{\mathbf{w}} \mathcal{J} = \frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \left(\frac{\partial \mathcal{J}}{\partial w_1}, \dots, \frac{\partial \mathcal{J}}{\partial w_D} \right) \quad (20)$$

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

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}} \quad (21)$$

- And for linear regression we have:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=0}^N (y^{(i)} - t^{(i)}) \mathbf{x}^{(i)} \quad (22)$$

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

Gradient Descent

- 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
 - Each GD update costs $O(ND)$
 - 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} :

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}} \quad (23)$$

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

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} (\mathcal{J} + \lambda \mathcal{R}) \quad (24)$$

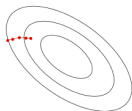
$$\mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} (\mathcal{J} + \lambda \mathcal{R}) = \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right) \quad (25)$$

$$\mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right) = \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \mathbf{w} \right) \quad (26)$$

$$\mathbf{w} \leftarrow (1 - \alpha \lambda) \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}} \quad (27)$$

Learning Rate (Step Size)

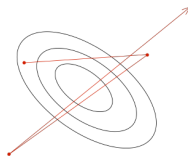
- In gradient descent, the learning rate α is a hyperparameter we need to tune. Here are some things that can go wrong:



α too small:
slow progress



α too large:
oscillations

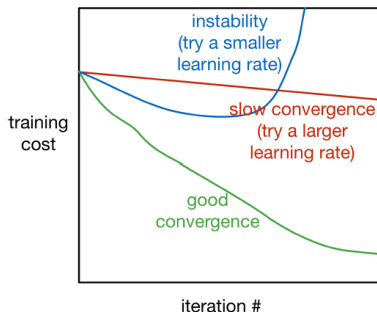


α much too large:
instability

- Good values are typically between 0.001 and 0.1. You should do a grid search if you want good performance.

Training Curve

- 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:

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N \mathcal{L}^{(i)} = \frac{1}{N} \sum_{i=1}^N \mathcal{L}(y(\mathbf{x}^{(i)}, \boldsymbol{\theta}), \mathbf{t}^{(i)}) \quad (28)$$

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

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}} = \frac{1}{N} \sum_{i=1}^N \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} \quad (29)$$

- 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,
 - Choose i uniformly at random;
 - $\theta \leftarrow \theta - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \theta}$
- 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:

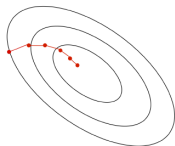
$$\mathbb{E} \left[\frac{\partial \mathcal{L}^{(i)}}{\partial \theta} \right] = \frac{1}{N} \sum_{i=1}^N \frac{\partial \mathcal{L}^{(i)}}{\partial \theta} = \frac{\partial \mathcal{J}}{\partial \theta} \quad (30)$$

Stochastic Gradient Descent

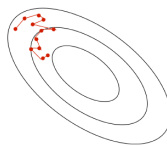
- Problems with using a single training example to estimate gradient:
 - Variance in the estimate may be high
 - We can't exploit efficient vectorized operations
- Compromise approach:
 - Compute the gradients on a randomly chosen medium-sized set of training $\mathcal{M} \subset \{1, \dots, N\}$ examples, called a mini-batch.
- Stochastic gradients computed on larger mini-batches have smaller variances.
- 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
 - 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

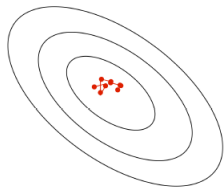


stochastic gradient descent

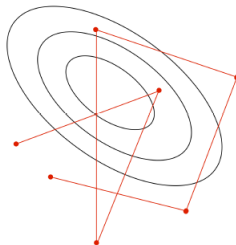
SDG Learning Rate

- In stochastic training, the learning rate also influences the fluctuations due to the stochasticity of the gradients.
- Stochasticity, in the context of machine learning, refers to the introduction of randomness or probabilistic elements into the learning process.

small learning rate

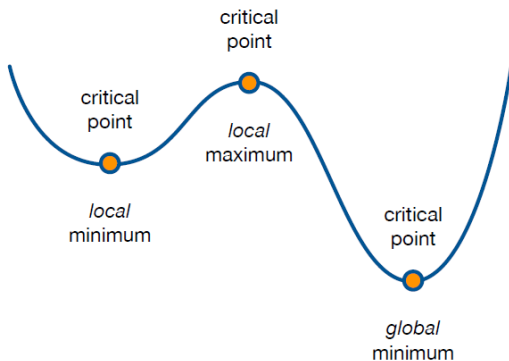


large learning rate



- 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.

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.