Gradient Descent Methods

Outline

Three Optimization Methods

Want to Minimize

$$RSS(\mathbf{w}) = ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 = \left\{\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\left(\mathbf{X}^\top \mathbf{y}\right)^\top \mathbf{w}\right\} + \text{const}$$

- Least-Squares Solution; taking the derivative and setting it to zero
- Batch Gradient Descent
- Stochastic Gradient Descent

Computational Complexity

Bottleneck of computing the solution?

$$\boldsymbol{w} = \left(\boldsymbol{X}^\top \boldsymbol{X}\right)^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

How many operations do we need?

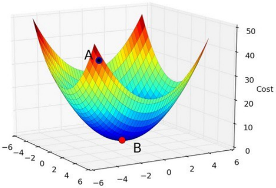
- $O(\mathrm{ND}^2)$ for matrix multiplication $\mathbf{X}^\top \mathbf{X}$
- $O(\mathrm{D}^3)$ (e.g., using Gauss-Jordan elimination) or $O(\mathrm{D}^{2.373})$ (recent theoretical advances) for matrix inversion of $\mathbf{X}^\top \mathbf{X}$
- $O(\mathrm{ND})$ for matrix multiplication $\mathbf{X}^\top \boldsymbol{y}$
- $O(\mathrm{D}^2)$ for $\left(\boldsymbol{X}^\top \boldsymbol{X}\right)^{-1}$ times $\boldsymbol{X}^\top \boldsymbol{y}$

$O(\mathrm{ND}^2) + O(\mathrm{D}^3)$ – Impractical for very large D or N

Alternative Method: Batch Gradient Descent

(Batch) Gradient Descent

- Initialize $\mathbf{w}$ to $\boldsymbol{w}^{(0)}$ (e.g., randomly); set $t = 0$; choose $\eta > 0$
- Loop *until convergence*
    1. Compute the gradient $\nabla RSS(\boldsymbol{w}) = \mathbf{X}^\top(\mathbf{X}\boldsymbol{w}^{(t)} - \boldsymbol{y})$
    2. Update the parameters $\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \nabla RSS(\boldsymbol{w})$
    3. $t \leftarrow t + 1$



What is the complexity of each iteration?
O(ND)

Why Would This Work?

If gradient descent converges, it will converge to the same solution as using matrix inversion.

This is because $RSS(\boldsymbol{w})$ is a convex function in its parameters $\boldsymbol{w}$.

Hessian of RSS

$$RSS(\boldsymbol{w}) = \boldsymbol{w}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{w} - 2\left(\mathbf{X}^\top \boldsymbol{y}\right)^\top \boldsymbol{w} + \text{const}$$
$$\Rightarrow \frac{\partial^2 RSS(\boldsymbol{w})}{\partial \boldsymbol{w}\boldsymbol{w}^\top} = 2\mathbf{X}^\top \mathbf{X}$$

$\mathbf{X}^\top \mathbf{X}$ is positive semidefinite, because for any $\boldsymbol{v}$

$$\boldsymbol{v}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{v} = \|\mathbf{X}^\top \boldsymbol{v}\|_2^2 \geq 0$$

Three Optimization Methods

Want to Minimize

$$RSS(\mathbf{w}) = ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 = \left\{\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\left(\mathbf{X}^\top \mathbf{y}\right)^\top \mathbf{w}\right\} + \text{const}$$

- Least-Squares Solution; taking the derivative and setting it to zero
- Batch Gradient Descent
- Stochastic Gradient Descent

Stochastic Gradient Descent (SGD)

Widrow-Hoff rule: update parameters using one example at a time

- Initialize $\boldsymbol{w}$ to some $\boldsymbol{w}^{(0)}$; set $t = 0$; choose $\eta > 0$
- Loop *until convergence*
  1. random choose a training a sample $\boldsymbol{x}_t$
  2. Compute its contribution to the gradient

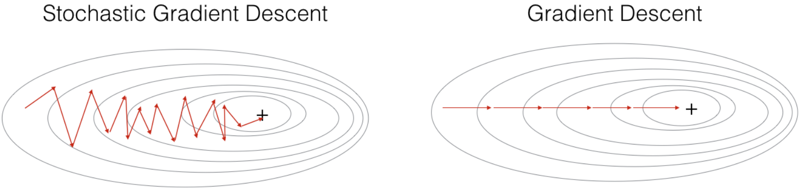
$$\boldsymbol{g}_t = (\boldsymbol{x}_t^\top \boldsymbol{w}^{(t)} - y_t)\mathbf{x}_t$$

  3. Update the parameters
     $\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \boldsymbol{g}_t$
  4. $t \leftarrow t + 1$

How does the complexity per iteration compare with gradient descent?

- $O(\mathrm{ND})$ for gradient descent versus $O(\mathrm{D})$ for SGD

SGD versus Batch GD



- SGD reduces per-iteration complexity from $O(\mathrm{ND})$ to $O(\mathrm{D})$
- But it is noisier and can take longer to converge

Example: Least Squares Solution

sqft (1000's)	sale price (100k)
1	2
2	3.5
1.5	3
2.5	4.5

The w_0 and w_1 that minimize this are given by:

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

$$\begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = \left(\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 1.5 & 2.5 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 1.5 \\ 1 & 2.5 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 1.5 & 2.5 \end{bmatrix} \begin{bmatrix} 2 \\ 3.5 \\ 3 \\ 4.5 \end{bmatrix}$$

$$\begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = \begin{bmatrix} 0.45 \\ 1.6 \end{bmatrix}$$

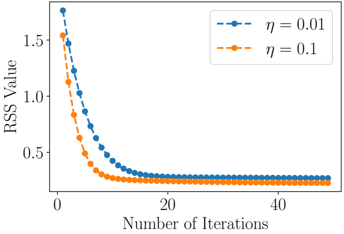
Minimum RSS is $RSS^* = ||\mathbf{X}\mathbf{w}^{LMS} - \mathbf{y}||_2^2 = 0.2236$

Example: Batch Gradient Descent

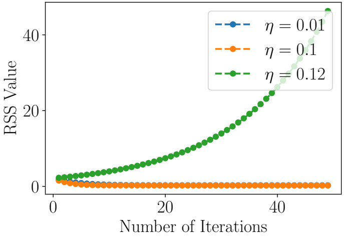
sqft (1000's)	sale price (100k)
1	2
2	3.5
1.5	3
2.5	4.5

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \nabla RSS(\boldsymbol{w}) = \boldsymbol{w}^{(t)} - \eta \mathbf{X}^\top \left(\mathbf{X}\boldsymbol{w}^{(t)} - \boldsymbol{y} \right)$$

Larger η gives faster convergence



But too large η makes GD unstable

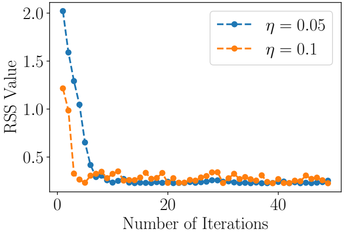


Example: Stochastic Gradient Descent

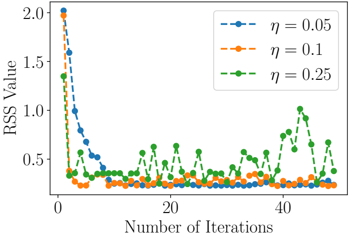
sqft (1000's)	sale price (100k)
1	2
2	3.5
1.5	3
2.5	4.5

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \nabla RSS(\boldsymbol{w}) = \boldsymbol{w}^{(t)} - \eta \left(\mathbf{x}_t^\top \boldsymbol{w}^{(t)} - \boldsymbol{y} \right) \mathbf{x}_t$$

Larger η gives faster convergence

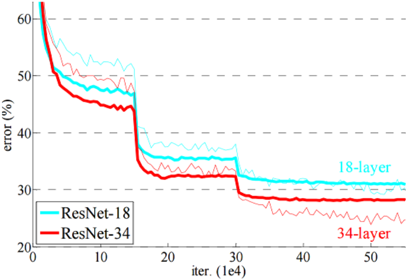


But too large η makes SGD unstable



How to Choose Learning Rate η in practice?

- Try $0.0001, 0.001, 0.01, 0.1$ etc. on a validation dataset (more on this later) and choose the one that gives fastest, stable convergence
- Reduce η by a constant factor (eg. 10) when learning saturates so that we can reach closer to the true minimum.
- More advanced learning rate schedules such as AdaGrad, Adam, AdaDelta are used in practice.



Summary of Gradient Descent Methods

- Batch gradient descent computes the exact gradient.
- Stochastic gradient descent approximates the gradient with a single data point; its expectation equals the true gradient.
- Mini-batch variant: set the batch size to trade-off between accuracy of estimating gradient and computational cost
- Similar ideas extend to other ML optimization problems.

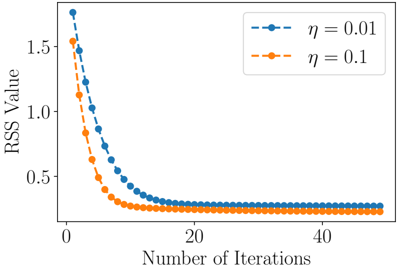
Feature Scaling

Outline

Batch Gradient Descent: Scaled Features

sqft (1000's)	sale price (100k)
1	2
2	3.5
1.5	3
2.5	4.5

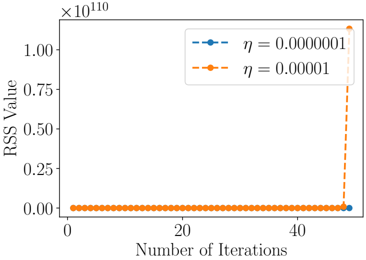
$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \nabla RSS(\boldsymbol{w}) = \boldsymbol{w}^{(t)} - \eta \mathbf{X}^\top \left(\mathbf{X} \boldsymbol{w}^{(t)} - \boldsymbol{y} \right)$$



Batch Gradient Descent: Without Feature Scaling

sqft	sale price
1000	200,000
2000	350,000
1500	300,000
2500	450,000

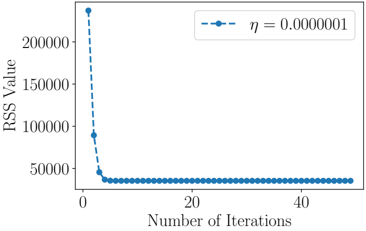
- Least-squares solution is $(w_0^*, w_1^*) = (45000, 160)$
- $\nabla RSS(\boldsymbol{w}^{(t)}) = \mathbf{X}^\top \left(\mathbf{X}\boldsymbol{w}^{(t)} - \boldsymbol{y}\right)$ becomes HUGE, causing instability
- We need a tiny η to compensate, but this can cause numerical issues



Batch Gradient Descent: Without Feature Scaling

sqft	sale price
1000	200,000
2000	350,000
1500	300,000
2500	450,000

- Least-squares solution is $(w_0^*, w_1^*) = (45000, 160)$
- $\nabla RSS(\boldsymbol{w})$ becomes HUGE, causing instability
- We need a tiny η to compensate, but this leads to slow convergence



How to Scale Features?

- **Min-max normalization**

$$x'_d = \frac{x_d - \min_n(x_d)}{\max_n x_d - \min_n x_d}$$

The min and max are taken over the possible values $x_d^{(1)}, \ldots x_d^{(N)}$ of x_d in the dataset. This will result in all scaled features $0 \leq x_d \leq 1$

- **Mean normalization**

$$x'_d = \frac{x_d - \text{avg}(x_d)}{\max_n x_d - \min_n x_d}$$

This will result in all scaled features $-1 \leq x_d \leq 1$

Labels $y^{(1)}, \ldots y^{(N)}$ should be similarly re-scaled

Several other methods: e.g., dividing by standard deviation (Z-score normalization)

Ridge Regression

Outline

What if $X^\top X$ Is Not Invertible?

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

Why might this happen?

- **Answer 1:** $\mathrm{N} < \mathrm{D}$. Not enough data to estimate all parameters. $\mathbf{X}^\top \mathbf{X}$ is not full-rank
- **Answer 2:** Columns of $\boldsymbol{X}$ are not linearly independent, e.g., some features are linear functions of other features. In this case, solution is not unique. Examples:
    - A feature is a re-scaled version of another, for example, having two features correspond to length in meters and feet respectively
    - Same feature is repeated twice (e.g., when there are many features)
    - A feature has the same value for all data points
    - A feature is a linear combination of others, such as the sum of two features being equal to a third feature

Example: Matrix $X^\top X$ Is Not Invertible

sqft (1000's)	bathrooms	sale price (100k)
1	2	2
2	2	3.5
1.5	2	3
2.5	2	4.5

Design matrix and target vector:

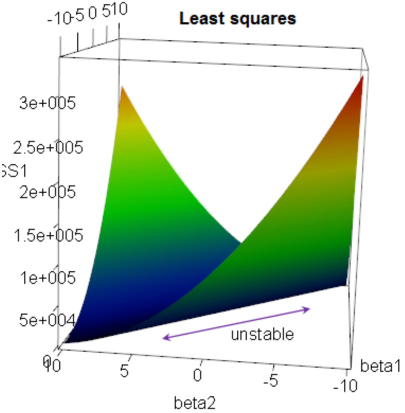
$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 2 \\ 1 & 1.5 & 2 \\ 1 & 2.5 & 2 \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 2 \\ 3.5 \\ 3 \\ 4.5 \end{bmatrix}$$

The 'bathrooms' feature is redundant, so we don't need w_2

$$\begin{aligned} y &= w_0 + w_1 x_1 + w_2 x_2 \\ &= w_0 + w_1 x_1 + w_2 \times 2, \quad \text{since } x_2 \text{ is always 2!} \\ &= w_{0,eff} + w_1 x_1, \quad \text{where } w_{0,eff} = (w_0 + 2w_2) \end{aligned}$$

What Does the RSS Look Like?

- When $\boldsymbol{X}^\top \boldsymbol{X}$ is not invertible, the RSS objective function has a ridge, that is, the minimum is a line instead of a single point



In our example, this line is $w_{0,eff} = (w_0 + 2w_2)$

How Do You Fix This Issue?

sqft (1000's)	bathrooms	sale price (100k)
1	2	2
2	2	3.5
1.5	2	3
2.5	2	4.5

- Manually remove redundant features
- But this can be tedious and non-trivial, especially when a feature is a linear combination of several other features

Need a general way that doesn't require manual feature engineering
SOLUTION: Ridge Regression

Ridge Regression

Intuition: what does a non-invertible $\boldsymbol{X}^\top \boldsymbol{X}$ mean?

Consider the EVD (why does this exist?) of this matrix:

$$\boldsymbol{X}^\top \boldsymbol{X} = \boldsymbol{V} \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & \lambda_r & 0 \\ 0 & \cdots & \cdots & 0 & 0 \end{bmatrix} \boldsymbol{V}^\top$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_r > 0$ and $r <$ D. We will have a divide by zero issue when computing $(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$...

Fix the problem: ensure all singular values are non-zero:

$$\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I} = \boldsymbol{V} \text{diag}(\lambda_1 + \lambda, \lambda_2 + \lambda, \cdots, \lambda) \boldsymbol{V}^\top$$

where $\lambda > 0$ and $\boldsymbol{I}$ is the identity matrix.

Regularized Least Squares (Ridge Regression)

Solution

$$\boldsymbol{w} = \left(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

This is equivalent to adding an extra term to $RSS(\boldsymbol{w})$

$$\overbrace{\frac{1}{2}\left\{\boldsymbol{w}^\top \boldsymbol{X}^\top \boldsymbol{X} \boldsymbol{w} - 2\left(\boldsymbol{X}^\top \boldsymbol{y}\right)^\top \boldsymbol{w} + \text{const.}\right\}}^{RSS(\boldsymbol{w})} + \underbrace{\frac{1}{2}\lambda \|w\|_2^2}_{\text{regularization}}$$

$$\frac{1}{2}\left\{\boldsymbol{w}^\top \left(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}\right) \boldsymbol{w} - 2\left(\boldsymbol{X}^\top \boldsymbol{y}\right)^\top \boldsymbol{w} + \text{const.}\right\}$$

Benefits

- Numerically more stable, invertible matrix
- Force **w** to be small
- Prevent overfitting — more on this in the next lecture

Ridge Regression on Our Example

sqft (1000's)	bathrooms	sale price (100k)
1	2	2
2	2	3.5
1.5	2	3
2.5	2	4.5

The 'bathrooms' feature is redundant, so we don't need w_2

$$\begin{aligned} y &= w_0 + w_1 x_1 + w_2 x_2 \\ &= w_0 + w_1 x_1 + w_2 \times 2, && \text{since } x_2 \text{ is always 2!} \\ &= w_{0,eff} + w_1 x_1, && \text{where } w_{0,eff} = (w_0 + 2w_2) \\ &= 0.45 + 1.6 x_1 && \text{Should get this} \end{aligned}$$

Ridge Regression on Our Example

The 'bathrooms' feature is redundant, so we don't need w_2

$$
\begin{aligned}
y &= w_0 + w_1 x_1 + w_2 x_2 \\
&= w_0 + w_1 x_1 + w_2 \times 2, \quad \text{since } x_2 \text{ is always 2!} \\
&= w_{0,eff} + w_1 x_1, \quad \text{where } w_{0,eff} = (w_0 + 2w_2) \\
&= 0.45 + 1.6 x_1 \quad \text{Should get this}
\end{aligned}
$$

Compute the solution for $\lambda = 0.5$

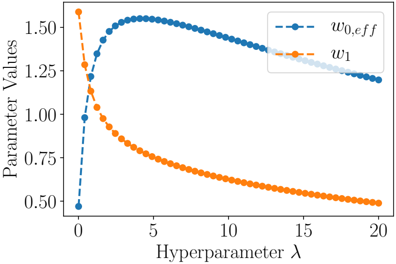
$$
\begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \left(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^\top \boldsymbol{y}
$$

$$
\begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0.208 \\ 1.247 \\ 0.4166 \end{bmatrix} \quad \text{recall} \quad \begin{bmatrix} w_{0,eff} \\ w_1 \end{bmatrix} = \begin{bmatrix} 0.45 \\ 1.6 \end{bmatrix} \text{ for LMS}
$$

How Does λ Affect the Solution?

$$\begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \left(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

Let us plot $w_{0,eff} = w_0 + 2w_2$ and w_1 for different $\lambda \in [0.01, 20]$

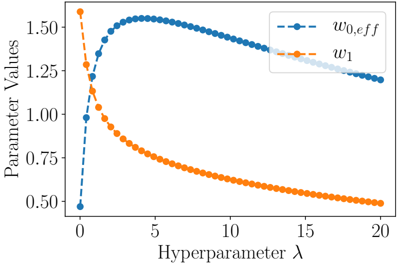


Setting small λ gives almost the least-squares solution, but it can cause numerical instability in the inversion

How to Choose λ?

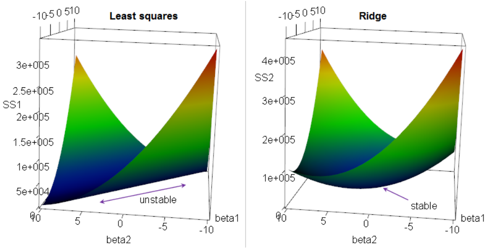
λ is referred to as a *hyperparameter*

- Associated with the estimation method, not the dataset
- In contrast, $\boldsymbol{w}$ is the parameter vector
- Use validation set or cross-validation to find good choice of λ (more on this in the next lecture)



Why Is It Called Ridge Regression?

- When $\boldsymbol{X}^\top \boldsymbol{X}$ is not invertible, the RSS objective function has a ridge, that is, the minimum is a line instead of a single point
- Adding the regularizer term $\frac{1}{2}\lambda\|w\|_2^2$ yields a unique minimum, thus avoiding instability in matrix inversion



Probabilistic Interpretation of Ridge Regression

Add a term to the objective function.

- Choose the parameters to not just minimize risk (i.e., minimize the RSS), but also avoid being too large.

$$\frac{1}{2}\left\{\boldsymbol{w}^\top \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} - 2\left(\boldsymbol{X}^\top \boldsymbol{y}\right)^\top \boldsymbol{w}\right\} + \frac{1}{2}\lambda\|w\|_2^2$$

Probabilistic interpretation: Place a prior on our weights

- Interpret $\boldsymbol{w}$ as a random variable
- Assume that each w_d is centered around zero
- Use observed data $\mathcal{D}$ to update our prior belief on $\boldsymbol{w}$

Gaussian priors lead to ridge regression.

Review: Probabilistic Interpretation of Linear Regression

Linear Regression model: $Y = \boldsymbol{w}^\top \boldsymbol{X} + \eta$
$\eta \sim N(0, \sigma_0^2)$ is a Gaussian random variable and $Y \sim N(\boldsymbol{w}^\top \boldsymbol{X}, \sigma_0^2)$

Frequentist interpretation: We assume that $\boldsymbol{w}$ is fixed.

- The likelihood function maps parameters to probabilities

$$L : \boldsymbol{w}, \sigma_0^2 \mapsto p(\mathcal{D}|\boldsymbol{w}, \sigma_0^2) = p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w}, \sigma_0^2) = \prod_n p(y_n|\boldsymbol{x}_n, \boldsymbol{w}, \sigma_0^2)$$

- Maximizing the likelihood with respect to $\boldsymbol{w}$ minimizes the RSS and yields the LMS solution:

$$\boldsymbol{w}^{\mathrm{LMS}} = \boldsymbol{w}^{\mathrm{ML}} = \arg\max_{\boldsymbol{w}} L(\boldsymbol{w}, \sigma_0^2)$$

Probabilistic Interpretation of Ridge Regression

Ridge Regression model: $Y = \boldsymbol{w}^\top \boldsymbol{X} + \eta$

- $Y \sim N(\boldsymbol{w}^\top \boldsymbol{X}, \sigma_0^2)$ is a Gaussian random variable (as before)
- $w_d \sim N(0, \sigma^2)$ are i.i.d. Gaussian random variables (unlike before)
- Note that all w_d share the same variance σ^2

- To find $\boldsymbol{w}$ given data $\mathcal{D}$, compute the posterior distribution of $\boldsymbol{w}$:

$$p(\boldsymbol{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w})}{p(\mathcal{D})}$$

- Maximum a posterior (MAP) estimate:

$$\boldsymbol{w}^{\mathrm{MAP}} = \arg\max_{\boldsymbol{w}} p(\boldsymbol{w}|\mathcal{D}) = \arg\max_{\boldsymbol{w}} p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w})$$

Estimating w

Let $\mathbf{x}_1, \ldots, \mathbf{x}_N$ be i.i.d. with $y|\boldsymbol{w}, \boldsymbol{x} \sim N(\boldsymbol{w}^\top \boldsymbol{x}, \sigma_0^2)$; $w_d \sim N(0, \sigma^2)$.

Joint likelihood of data and parameters (given σ_0, σ):

$$p(\mathcal{D}, \boldsymbol{w}) = p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w}) \quad = \prod_n p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) \prod_d p(w_d)$$

Plugging in the Gaussian PDF, we get:

$$\begin{aligned}\log p(\mathcal{D}, \boldsymbol{w}) &= \sum_n \log p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) + \sum_d \log p(w_d) \\ &= -\frac{\sum_n (\boldsymbol{w}^\top \boldsymbol{x}_n - y_n)^2}{2\sigma_0^2} - \sum_d \frac{1}{2\sigma^2} w_d^2 + \text{const}\end{aligned}$$

MAP estimate: $\boldsymbol{w}^{\mathrm{MAP}} = \arg\max_{\boldsymbol{w}} \log p(\mathcal{D}, \boldsymbol{w})$

$$\boldsymbol{w}^{\mathrm{MAP}} = \operatorname{argmin}_{\boldsymbol{w}} \left\{ \frac{\sum_n (\boldsymbol{w}^\top \boldsymbol{x}_n - y_n)^2}{2\sigma_0^2} + \frac{1}{2\sigma^2} \|\boldsymbol{w}\|_2^2 \right\}$$

Maximum a Posteriori (MAP) Estimate

MAP Estimate:

$$\boldsymbol{w}^{\mathrm{MAP}} = \operatorname{argmin}_{\boldsymbol{w}} \left\{ \frac{\sum_n (\boldsymbol{w}^\top \boldsymbol{x}_n - y_n)^2}{2\sigma_0^2} + \frac{1}{2\sigma^2} \|\boldsymbol{w}\|_2^2 \right\}$$

After multiplying by $2\sigma_0^2$:

$$\boldsymbol{w}^{\mathrm{MAP}} = \operatorname{argmin}_{\boldsymbol{w}} \left\{ \underbrace{\sum_n (\boldsymbol{w}^\top \boldsymbol{x}_n - y_n)^2}_{RSS} + \frac{\sigma_0^2}{\sigma^2} \underbrace{\|\boldsymbol{w}\|_2^2}_{regularizer} \right\}$$

which is the same as our ridge regression formulation if we define $\lambda = \sigma_0^2 / \sigma^2 > 0$. This extra term $\|\boldsymbol{w}\|_2^2$ is called regularization/regularizer and controls the magnitude of $\boldsymbol{w}$.

What Does the MAP Estimate Tell Us?

$$\mathcal{E}(\boldsymbol{w}) = \sum_n (\boldsymbol{w}^\top \boldsymbol{x}_n - y_n)^2 + \lambda \|\boldsymbol{w}\|_2^2$$

where $\lambda > 0$ is used to denote σ_0^2/σ^2.

Intuitions

- If $\lambda \to +\infty$, then $\sigma_0^2 \gg \sigma^2$: the variance of noise is far greater than what our prior model can allow for $\boldsymbol{w}$. In this case, our prior model on $\boldsymbol{w}$ will force $\boldsymbol{w}$ to be close to zero. Numerically,

$$\boldsymbol{w}^{\mathrm{MAP}} \to \mathbf{0}$$

- If $\lambda \to 0$, then we trust our data more. Numerically,

$$\boldsymbol{w}^{\mathrm{MAP}} \to \boldsymbol{w}^{\mathrm{LMS}} = \operatorname{argmin} \sum_n (\boldsymbol{w}^\top \boldsymbol{x}_n - y_n)^2$$

Outline

1. Review of Linear Regression
2. Gradient Descent Methods
3. Feature Scaling
4. Ridge Regression
5. Non-linear Basis Functions

Non-linear Basis Functions

Outline

Review of Linear Regression

Gradient Descent Methods

Feature Scaling

Ridge Regression

Non-linear Basis Functions

Should We Always Use a Linear Model?

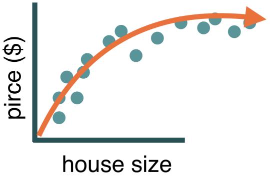


Figure 1: Sale price can saturate as square footage increases

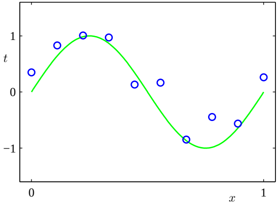


Figure 2: Temperature has cyclic variations over each year

General Nonlinear Basis Functions

We can use a nonlinear mapping to a new feature vector:

$$\phi(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^D \rightarrow \boldsymbol{z} \in \mathbb{R}^M$$

- M is dimensionality of new features $\boldsymbol{z}$ (or $\phi(\boldsymbol{x})$)
- M could be greater than, less than, or equal to D

We can apply existing learning methods on the transformed data:

- linear methods: prediction is based on $\boldsymbol{w}^\top \phi(\boldsymbol{x})$
- other methods: nearest neighbors, decision trees, etc

Regression with Nonlinear Basis

Residual sum of squares

$$\sum_n [\boldsymbol{w}^\top \phi(\boldsymbol{x}_n) - y_n]^2$$

where $\boldsymbol{w} \in \mathbb{R}^M$, the same dimensionality as the transformed features $\phi(\boldsymbol{x})$.

The LMS solution can be formulated with the new design matrix

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi(\boldsymbol{x}_1)^\top \\ \phi(\boldsymbol{x}_2)^\top \\ \vdots \\ \phi(\boldsymbol{x}_N)^\top \end{pmatrix} \in \mathbb{R}^{N \times M}, \quad \boldsymbol{w}^{\mathrm{LMS}} = \left(\boldsymbol{\Phi}^\top \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^\top \boldsymbol{y}$$

Example: Flexibility in Designing New Features!

x_1, Area (1k sqft)	x_1^2, Area^2	Price (100k)
1	1	2
2	4	3.5
1.5	2.25	3
2.5	6.25	4.5

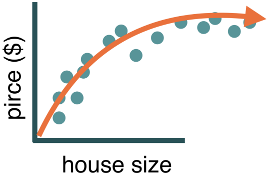


Figure 3: Add x_1^2 as a feature to allow us to fit quadratic, instead of linear functions of the house area x_1

Example: Flexibility in Designing New Features!

x_1, front (100ft)	x_2 depth (100ft)	$10x_1x_2$, Lot (1k sqft)	Price (100k)
0.5	0.5	2.5	2
0.5	1	5	3.5
0.8	1.5	12	3
1.0	1.5	15	4.5

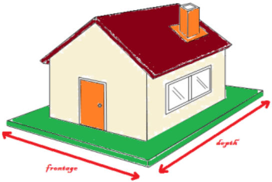


Figure 4: Instead of having frontage and depth as two separate features, it may be better to consider the lot-area, which is equal to frontage×depth

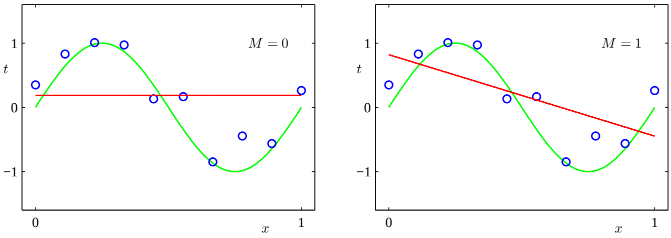
Example with Regression

Polynomial basis functions

$$\phi(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^M \end{bmatrix} \Rightarrow f(x) = w_0 + \sum_{m=1}^{M} w_m x^m$$

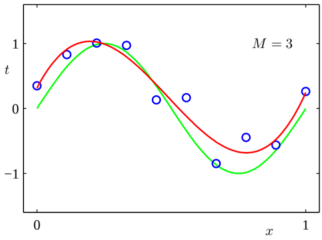
Fitting samples from a sine function:

underfitting since $f(x)$ is too simple

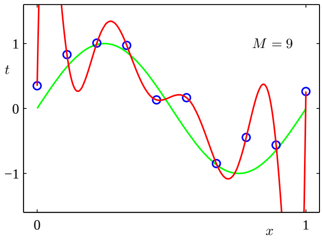


Adding Higher-order Terms

M=3



M=9: overfitting



More complex features lead to better results on the training data, but potentially worse results on new data, e.g., test data!

You Should Know

- Advantages and disadvantages of the least-mean-squares, batch gradient descent, and stochastic gradient descent solution methods
- Examples of feature scaling and why it can be important
- Formulation and solution of ridge regression
- Probabilistic interpretation of ridge regression
- How to use nonlinear basis functions in linear regression