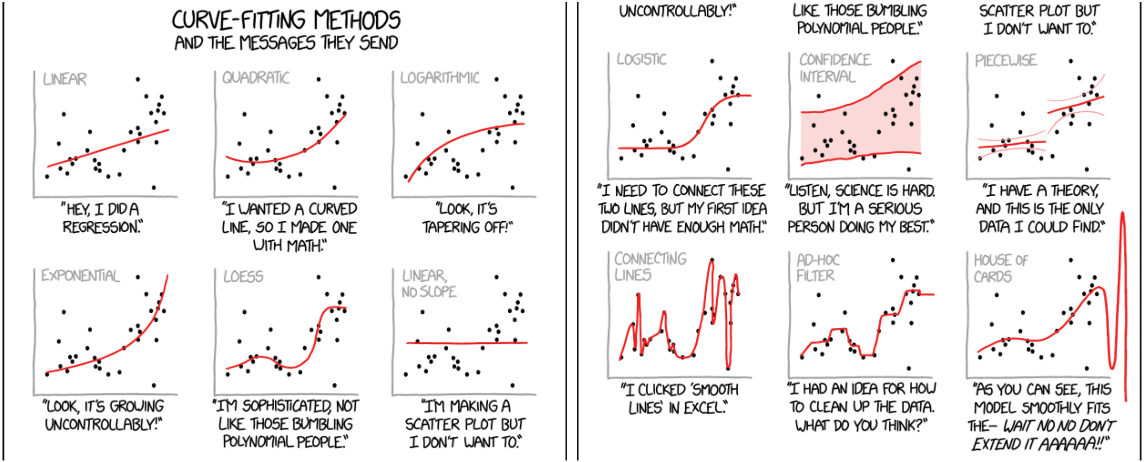

CURVE-FITTING METHODS
AND THE MESSAGES THEY SEND
LINEAR
"HEY, I DID A REGRESSION."
QUADRATIC
"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."
LOGARITHMIC
"LOOK, IT'S TAPERING OFF!"
EXPONENTIAL
"LOOK, IT'S GROWING UNCONTROLLABLY!"
LOESS
"I'M SOPHISTICATED, NOT LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."
LINEAR, NO SLOPE
"I'M MAKING A SCATTER PLOT BUT I DON'T WANT TO."
UNCONTROLLABLY!"
LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."
SCATTER PLOT BUT I DON'T WANT TO."
LOGISTIC
"I NEED TO CONNECT THESE TWO LINES, BUT MY FIRST IDEA DIDN'T HAVE ENOUGH MATH."
CONFIDENCE INTERVAL
"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."
PIECEWISE
"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."
CONNECTING LINES
"I CLICKED 'SMOOTH LINES' IN EXCEL."
AD-HOC FILTER
"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"
HOUSE OF CARDS
"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE– WAIT NO NO DON'T EXTEND IT AAAAAA!!"

Controling Complexity: Feature Selection and Regularization

CDS, NYU

Feb 7, 2022

Complexity of Hypothesis Spaces

What is the trade-off between approximation error and estimation error?

Complexity of Hypothesis Spaces

What is the trade-off between approximation error and estimation error?

- Bigger $\mathcal{F}$: better approximation but can overfit (need more samples)
- Smaller $\mathcal{F}$: less likely to overfit but can be farther from the true function

Complexity of Hypothesis Spaces

What is the trade-off between approximation error and estimation error?

- Bigger $\mathcal{F}$: better approximation but can overfit (need more samples)
- Smaller $\mathcal{F}$: less likely to overfit but can be farther from the true function

To control the "size" of $\mathcal{F}$, we need some measure of its complexity:

- Number of variables / features
- Degree of polynomial

General Approach to Control Complexity

1. Learn a sequence of models varying in complexity from the training data

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$$

General Approach to Control Complexity

1. Learn a sequence of models varying in complexity from the training data

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$$

   Example: Polynomial Functions

   - $\mathcal{F} = \{\text{all polynomial functions}\}$
   - $\mathcal{F}_d = \{\text{all polynomials of degree } \leqslant d\}$

General Approach to Control Complexity

1. Learn a sequence of models varying in complexity from the training data

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$$

   Example: Polynomial Functions

   - $\mathcal{F} = \{\text{all polynomial functions}\}$
   - $\mathcal{F}_d = \{\text{all polynomials of degree } \leqslant d\}$

2. Select one of these models based on a score (e.g. validation error)

Feature Selection in Linear Regression

Nested sequence of hypothesis spaces: $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$

- $\mathcal{F} = \{$linear functions using all features$\}$
- $\mathcal{F}_d = \{$linear functions using fewer than d features$\}$

Feature Selection in Linear Regression

Nested sequence of hypothesis spaces: $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$

- $\mathcal{F} = \{$linear functions using all features$\}$
- $\mathcal{F}_d = \{$linear functions using fewer than d features$\}$

Best subset selection:

- Choose the subset of features that is best according to the score (e.g. validation error)
  - Example with two features: Train models using $\{\}$, $\{X_1\}$, $\{X_2\}$, $\{X_1, X_2\}$, respectively
- Not an efficient search algorithm; iterating over all subsets becomes very expensive with a large number of features

Greedy Selection Methods

Forward selection:

1. Start with an empty set of features S

Greedy Selection Methods

Forward selection:

1. Start with an empty set of features S
2. For each feature i not in S
   - Learn a model using features $S \cup i$
   - Compute score of the model: α_i

Greedy Selection Methods

Forward selection:

1. Start with an empty set of features S
2. For each feature i not in S
   - Learn a model using features $S \cup i$
   - Compute score of the model: α_i
3. Find the candidate feature with the highest score: $j = \arg\max_i \alpha_i$

Greedy Selection Methods

Forward selection:

1. Start with an empty set of features S
2. For each feature i not in S
   - Learn a model using features $S \cup i$
   - Compute score of the model: α_i
3. Find the candidate feature with the highest score: $j = \arg\max_i \alpha_i$
4. If α_j improves the current best score, add feature j: $S \leftarrow S \cup j$ and go to step 2; return S otherwise.

Greedy Selection Methods

Forward selection:

1. Start with an empty set of features S
2. For each feature i not in S
   - Learn a model using features $S \cup i$
   - Compute score of the model: α_i
3. Find the candidate feature with the highest score: $j = \arg\max_i \alpha_i$
4. If α_j improves the current best score, add feature j: $S \leftarrow S \cup j$ and go to step 2; return S otherwise.

Backward Selection:

- Start with all features; in each iteration, remove the worst feature

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function
- General approach to feature selection:

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function
- General approach to feature selection:
  - Define a score that balances training error and complexity

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function
- General approach to feature selection:
  - Define a score that balances training error and complexity
  - Find the subset of features that maximizes the score

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function
- General approach to feature selection:
  - Define a score that balances training error and complexity
  - Find the subset of features that maximizes the score
- Forward & backward selection do not guarantee to find the best solution.

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function
- General approach to feature selection:
    - Define a score that balances training error and complexity
    - Find the subset of features that maximizes the score
- Forward & backward selection do not guarantee to find the best solution.
- Forward & backward selection do not in general result in the same subset.

ℓ_2 and ℓ_1 Regularization

Complexity Penalty

An objective that balances number of features and prediction performance:

$$\text{score}(S) = \text{training\_loss}(S) + \lambda |S| \tag{1}$$

Complexity Penalty

An objective that balances number of features and prediction performance:

$$\text{score}(S) = \text{training\_loss}(S) + \lambda |S| \tag{1}$$

λ balances the training loss and the number of features used:

- Adding an extra feature must be justified by at least λ improvement in training loss
- Larger $\lambda \to$ complex models are penalized more heavily

Complexity Penalty

Goal: Balance the complexity of the hypothesis space $\mathcal{F}$ and the training loss

Complexity measure: $\Omega : \mathcal{F} \to [0, \infty)$, e.g. number of features

Complexity Penalty

Goal: Balance the complexity of the hypothesis space $\mathcal{F}$ and the training loss

Complexity measure: $\Omega : \mathcal{F} \to [0, \infty)$, e.g. number of features

Penalized ERM (Tikhonov regularization)

For complexity measure $\Omega : \mathcal{F} \to [0, \infty)$ and fixed $\lambda \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \Omega(f)$$

As usual, we find λ using the validation data.

Complexity Penalty

Goal: Balance the complexity of the hypothesis space $\mathcal{F}$ and the training loss

Complexity measure: $\Omega : \mathcal{F} \to [0, \infty)$, e.g. number of features

Penalized ERM (Tikhonov regularization)

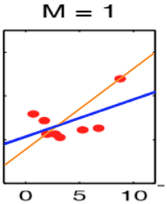
For complexity measure $\Omega : \mathcal{F} \to [0, \infty)$ and fixed $\lambda \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \Omega(f)$$

As usual, we find λ using the validation data.

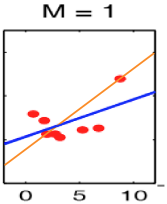
Number of features as complexity measure is hard to optimize—other measures?

Weight Shrinkage: Intuition



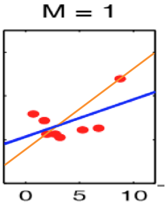
- Why would we prefer a regression line with smaller slope (unless the data strongly supports a larger slope)?

Weight Shrinkage: Intuition



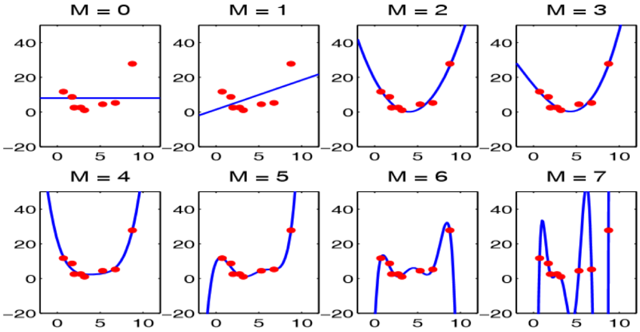
- Why would we prefer a regression line with smaller slope (unless the data strongly supports a larger slope)?
- More conservative: small change in the input does not cause large change in the output

Weight Shrinkage: Intuition



- Why would we prefer a regression line with smaller slope (unless the data strongly supports a larger slope)?
- More conservative: small change in the input does not cause large change in the output
- If we push the estimated weights to be small, re-estimating them on a new dataset wouldn't cause the prediction function to change dramatically (less sensitive to noise in data)

Weight Shrinkage: Polynomial Regression



- Large weights are needed to make the curve wiggle sufficiently to overfit the data
- $\hat{y} = 0.001x^7 + 0.003x^3 + 1$ less likely to overfit than $\hat{y} = 1000x^7 + 500x^3 + 1$

(Adapated from Mark Schmidt's slide)

Linear Regression with ℓ_2 Regularization

- We have a linear model

$$\mathcal{F} = \left\{ f : \mathrm{R}^d \to \mathrm{R} \mid f(x) = w^T x \text{ for } w \in \mathrm{R}^d \right\}$$

- Square loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- Training data $\mathcal{D}_n = \left((x_1, y_1), \ldots, (x_n, y_n) \right)$

Linear Regression with ℓ_2 Regularization

- We have a linear model

$$\mathcal{F} = \left\{ f : \mathbb{R}^d \to \mathbb{R} \mid f(x) = w^T x \text{ for } w \in \mathbb{R}^d \right\}$$

- Square loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- Training data $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$
- Linear least squares regression is ERM for square loss over $\mathcal{F}$:

$$\hat{w} = \underset{w \in \mathbb{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left(w^T x_i - y_i \right)^2$$

- This often overfits, especially when d is large compared to n (e.g. in NLP one can have 1M features for 10K documents).

Linear Regression with L2 Regularization

Penalizes large weights:

$$\hat{w} = \arg\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2,$$

where $\|w\|_2^2 = w_1^2 + \cdots + w_d^2$ is the square of the ℓ_2-norm.

- Also known as **ridge regression**.

Linear Regression with L2 Regularization

Penalizes large weights:

$$\hat{w} = \underset{w \in \mathrm{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2,$$

where $\|w\|_2^2 = w_1^2 + \cdots + w_d^2$ is the square of the ℓ_2-norm.

- Also known as **ridge regression**.
- Equivalent to linear least square regression when $\lambda = 0$.

Linear Regression with L2 Regularization

Penalizes large weights:

$$\hat{w} = \underset{w \in \mathbb{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2,$$

where $\|w\|_2^2 = w_1^2 + \cdots + w_d^2$ is the square of the ℓ_2-norm.

- Also known as **ridge regression**.
- Equivalent to linear least square regression when $\lambda = 0$.
- ℓ_2 regularization can be used for other models too (e.g. neural networks).

ℓ_2 regularization reduces sensitivity to changes in input

- $\hat{f}(x) = \hat{w}^T x$ is **Lipschitz continuous** with Lipschitz constant $L = \|\hat{w}\|_2$: when moving from x to $x+h$, $\hat{f}$ changes no more than $L\|h\|$.

ℓ_2 regularization reduces sensitivity to changes in input

- $\hat{f}(x) = \hat{w}^T x$ is **Lipschitz continuous** with Lipschitz constant $L = \|\hat{w}\|_2$: when moving from x to $x + h$, $\hat{f}$ changes no more than $L\|h\|$.
- ℓ_2 regularization controls the maximum rate of change of $\hat{f}$.

ℓ_2 regularization reduces sensitivity to changes in input

- $\hat{f}(x) = \hat{w}^T x$ is **Lipschitz continuous** with Lipschitz constant $L = \|\hat{w}\|_2$: when moving from x to $x+h$, $\hat{f}$ changes no more than $L\|h\|$.
- ℓ_2 regularization controls the maximum rate of change of $\hat{f}$.
- Proof:

$$
\begin{aligned}
\left|\hat{f}(x+h) - \hat{f}(x)\right| &= |\hat{w}^T(x+h) - \hat{w}^T x| = \left|\hat{w}^T h\right| \\
&\leqslant \|\hat{w}\|_2 \|h\|_2 \quad \text{(Cauchy-Schwarz inequality)}
\end{aligned}
$$

ℓ_2 regularization reduces sensitivity to changes in input

- $\hat{f}(x) = \hat{w}^T x$ is **Lipschitz continuous** with Lipschitz constant $L = \|\hat{w}\|_2$: when moving from x to $x+h$, $\hat{f}$ changes no more than $L\|h\|$.
- ℓ_2 regularization controls the maximum rate of change of $\hat{f}$.
- Proof:

$$\begin{aligned}\left|\hat{f}(x+h) - \hat{f}(x)\right| &= |\hat{w}^T(x+h) - \hat{w}^T x| = \left|\hat{w}^T h\right| \\ &\leqslant \|\hat{w}\|_2\|h\|_2 \quad \text{(Cauchy-Schwarz inequality)}\end{aligned}$$

- Other norms also provide a bound on L due to the equivalence of norms: $\exists C > 0$ s.t. $\|\hat{w}\|_2 \leqslant C\|\hat{w}\|_p$

Linear Regression vs. Ridge Regression

Objective:

- Linear: $L(w) = \frac{1}{2}\|Xw - y\|_2^2$
- Ridge: $L(w) = \frac{1}{2}\|Xw - y\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$

Linear Regression vs. Ridge Regression

Objective:

- Linear: $L(w) = \frac{1}{2}\|Xw - y\|_2^2$
- Ridge: $L(w) = \frac{1}{2}\|Xw - y\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$

Gradient:

- Linear: $\nabla L(w) = X^T(Xw - y)$
- Ridge: $\nabla L(w) = X^T(Xw - y) + \lambda w$
    - Also known as **weight decay** in neural networks

Linear Regression vs. Ridge Regression

Objective:

- Linear: $L(w) = \frac{1}{2}\|Xw - y\|_2^2$
- Ridge: $L(w) = \frac{1}{2}\|Xw - y\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$

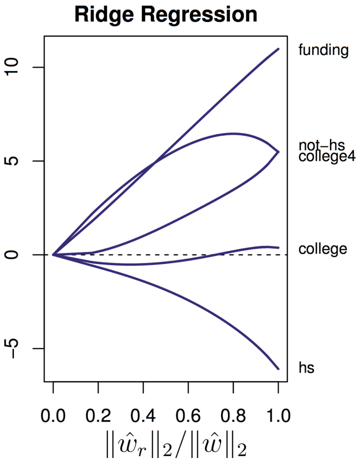
Gradient:

- Linear: $\nabla L(w) = X^T(Xw - y)$
- Ridge: $\nabla L(w) = X^T(Xw - y) + \lambda w$
    - Also known as **weight decay** in neural networks

Closed-form solution:

- Linear: $X^T X w = X^T y$
- Ridge: $(X^T X + \lambda I)w = X^T y$
    - $(X^T X + \lambda I)$ is always invertible

Ridge Regression: Regularization Path



$$\hat{w}_r = \underset{\|w\|_2^2 \le r^2}{\arg\min} \frac{1}{n}\sum_{i=1}^{n}\left(w^T x_i - y_i\right)^2$$
$$\hat{w} = \hat{w}_\infty = \text{Unconstrained ERM}$$

- For $r = 0$, $\|\hat{w}_r\|_2/\|\hat{w}\|_2 = 0$.
- For $r = \infty$, $\|\hat{w}_r\|_2/\|\hat{w}\|_2 = 1$

Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

Lasso Regression

Penalize the ℓ_1 norm of the weights:

Lasso Regression (Tikhonov Form, soft penalty)

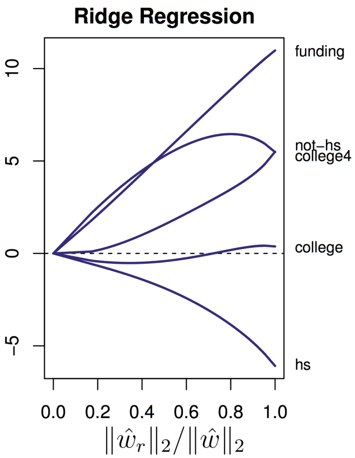
$$\hat{w} = \underset{w \in \mathbf{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_1,$$

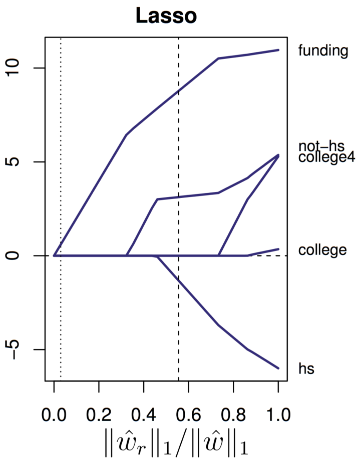
where $\|w\|_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1-norm.

("Least Absolute Shrinkage and Selection Operator")

Ridge vs. Lasso: Regularization Paths

Lasso yields sparse weights:





Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

The Benefits of Sparsity

The coefficient for a feature is 0 $\implies$ the feature is not needed for prediction. Why is that useful?

The Benefits of Sparsity

The coefficient for a feature is 0 $\implies$ the feature is not needed for prediction. Why is that useful?

- Faster to compute the features; cheaper to measure or annotate them

The Benefits of Sparsity

The coefficient for a feature is 0 $\implies$ the feature is not needed for prediction. Why is that useful?

- Faster to compute the features; cheaper to measure or annotate them
- Less memory to store features (deployment on a mobile device)

The Benefits of Sparsity

The coefficient for a feature is 0 $\implies$ the feature is not needed for prediction. Why is that useful?

- Faster to compute the features; cheaper to measure or annotate them
- Less memory to store features (deployment on a mobile device)
- Interpretability: identifies the important features

The Benefits of Sparsity

The coefficient for a feature is 0 $\implies$ the feature is not needed for prediction. Why is that useful?

- Faster to compute the features; cheaper to measure or annotate them
- Less memory to store features (deployment on a mobile device)
- Interpretability: identifies the important features
- Prediction function may generalize better (model is less complex)

Why does ℓ_1 Regularization Lead to Sparsity?

Regularization as Constrained Empirical Risk Minimization

Constrained ERM (Ivanov regularization)

For complexity measure $\Omega : \mathcal{F} \to [0, \infty)$ and fixed $r \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

$$\text{s.t. } \Omega(f) \leqslant r$$

Lasso Regression (Ivanov Form, hard constraint)

The lasso regression solution for complexity parameter $r \geqslant 0$ is

$$\hat{w} = \underset{\|w\|_1 \leqslant r}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 .$$

r has the same role as λ in penalized ERM (Tikhonov).

Ivanov vs. Tikhonov Regularization

- Let $L : \mathcal{F} \to \mathrm{R}$ be any performance measure of f
  - e.g. $L(f)$ could be the empirical risk of f

Ivanov vs. Tikhonov Regularization

- Let $L : \mathcal{F} \to \mathrm{R}$ be any performance measure of f
  - e.g. $L(f)$ could be the empirical risk of f
- For many L and Ω, Ivanov and Tikhonov are equivalent:
  - Any solution f^* we can get from Ivanov, we can also get from Tikhonov.
  - Any solution f^* we can get from Tikhonov, we can also get from Ivanov.

Ivanov vs. Tikhonov Regularization

- Let $L : \mathcal{F} \to \mathrm{R}$ be any performance measure of f
  - e.g. $L(f)$ could be the empirical risk of f
- For many L and Ω, Ivanov and Tikhonov are equivalent:
  - Any solution f^* we can get from Ivanov, we can also get from Tikhonov.
  - Any solution f^* we can get from Tikhonov, we can also get from Ivanov.
- The conditions for this equivalence can be derived from Lagrangian duality theory.

Ivanov vs. Tikhonov Regularization

- Let $L : \mathcal{F} \to \mathrm{R}$ be any performance measure of f
  - e.g. $L(f)$ could be the empirical risk of f
- For many L and Ω, Ivanov and Tikhonov are equivalent:
  - Any solution f^* we can get from Ivanov, we can also get from Tikhonov.
  - Any solution f^* we can get from Tikhonov, we can also get from Ivanov.
- The conditions for this equivalence can be derived from Lagrangian duality theory.
- In practice, both approaches are effective: we will use whichever one is more convenient for training or analysis.

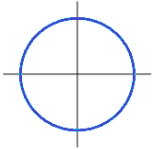
The ℓ_1 and ℓ_2 Norm Constraints

- Let's consider $\mathcal{F} = \{f(x) = w_1x_1 + w_2x_2\}$ space)
- We can represent each function in $\mathcal{F}$ as a point $(w_1, w_2) \in \mathrm{R}^2$.
- Where in R^2 are the functions that satisfy the Ivanov regularization constraint for ℓ_1 and ℓ_2?

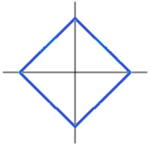
The ℓ_1 and ℓ_2 Norm Constraints

- Let's consider $\mathcal{F} = \{f(x) = w_1x_1 + w_2x_2\}$ space)
- We can represent each function in $\mathcal{F}$ as a point $(w_1, w_2) \in \mathrm{R}^2$.
- Where in R^2 are the functions that satisfy the Ivanov regularization constraint for ℓ_1 and ℓ_2?

- ℓ_2 contour:
  $w_1^2 + w_2^2 = r$



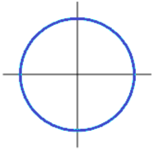
- ℓ_1 contour:
  $|w_1| + |w_2| = r$



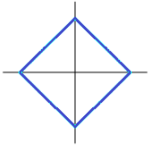
The ℓ_1 and ℓ_2 Norm Constraints

- Let's consider $\mathcal{F} = \{f(x) = w_1 x_1 + w_2 x_2\}$ space)
- We can represent each function in $\mathcal{F}$ as a point $(w_1, w_2) \in \mathbf{R}^2$.
- Where in $\mathbf{R}^2$ are the functions that satisfy the Ivanov regularization constraint for ℓ_1 and ℓ_2?

- ℓ_2 contour: $w_1^2 + w_2^2 = r$



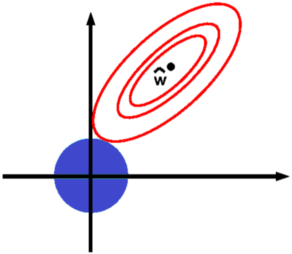
- ℓ_1 contour: $|w_1| + |w_2| = r$



- Where are the sparse solutions?

Visualizing Regularization

- $f_r^* = \arg\min_{w \in \mathbb{R}^2} \sum_{i=1}^n \left(w^T x_i - y_i\right)^2$ subject to $w_1^2 + w_2^2 \leqslant r$

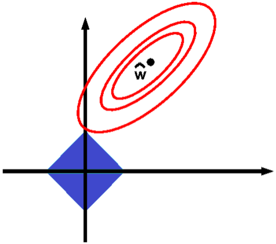


- Blue region: Area satisfying complexity constraint: $w_1^2 + w_2^2 \leqslant r$
- Red lines: contours of the empirical risk $\hat{R}_n(w) = \sum_{i=1}^n \left(w^T x_i - y_i\right)^2$.

KPM Fig. 13.3

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

- $f_r^* = \arg\min_{w \in \mathbf{R}^2} \frac{1}{n} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$ subject to $|w_1| + |w_2| \leqslant r$



- Blue region: Area satisfying complexity constraint: $|w_1| + |w_2| \leqslant r$
- Red lines: contours of the empirical risk $\hat{R}_n(w) = \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$.
- ℓ_1 solution tends to touch the corners.

KPM Fig. 13.3

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

Geometric intuition: Projection onto diamond encourages solutions at corners.

- $\hat{w}$ in red/green regions are closest to corners in the ℓ_1 "ball".

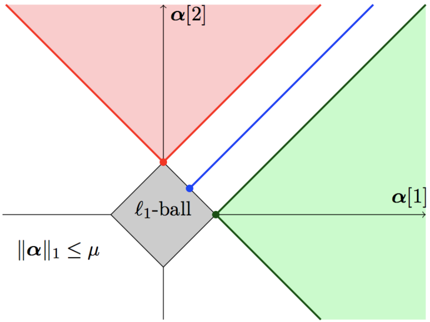


Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.6

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

Geometric intuition: Projection onto ℓ_2 sphere favors all directions equally.

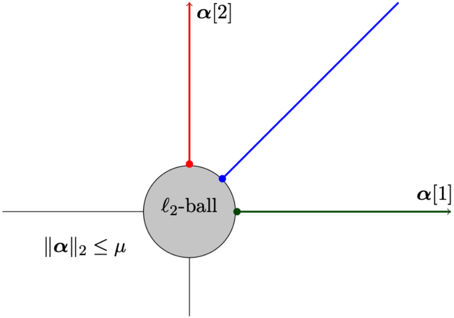


Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.6

Why does ℓ_2 Encourage Sparsity? Optimization Perspective

For ℓ_2 regularization,

- As w_i becomes smaller, there is less and less penalty
  - What is the ℓ_2 penalty for $w_i = 0.0001$?
- The gradient—which determines the pace of optimization—decreases as w_i approaches zero
- Less incentive to make a small weight equal to exactly zero

Why does ℓ_2 Encourage Sparsity? Optimization Perspective

For ℓ_2 regularization,

- As w_i becomes smaller, there is less and less penalty
  - What is the ℓ_2 penalty for $w_i = 0.0001$?
- The gradient—which determines the pace of optimization—decreases as w_i approaches zero
- Less incentive to make a small weight equal to exactly zero

For ℓ_1 regularization,

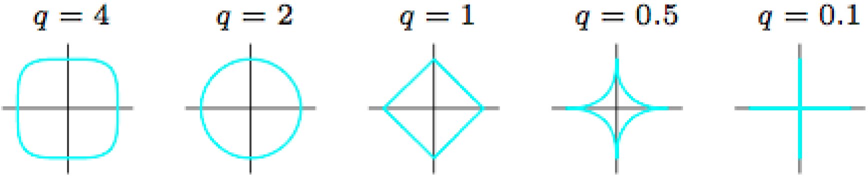
- The gradient stays the same as the weights approach zero
- This pushes the weights to be exactly zero even if they are already small

(ℓ_q) Regularization

- We can generalize to ℓ_q : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.

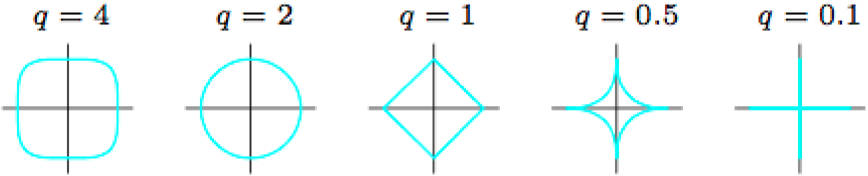
(ℓ_q) Regularization

- We can generalize to ℓ_q : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.



(ℓ_q) Regularization

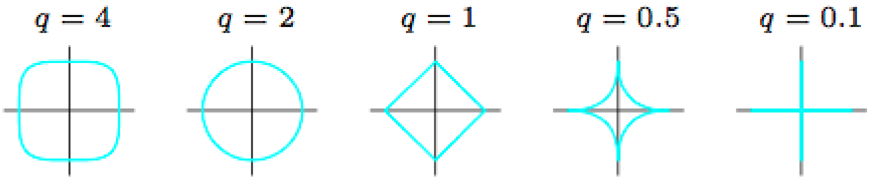
- We can generalize to ℓ_q : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.



- Note: $\|w\|_q$ is only a norm if $q \geqslant 1$, but not for $q \in (0, 1)$

(ℓ_q) Regularization

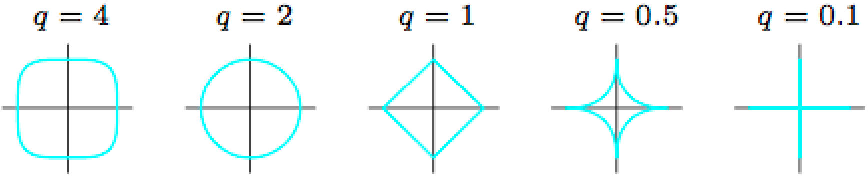
- We can generalize to ℓ_q : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.



- Note: $\|w\|_q$ is only a norm if $q \geqslant 1$, but not for $q \in (0, 1)$
- When $q < 1$, the ℓ_q constraint is non-convex, so it is hard to optimize; lasso is good enough in practice

(ℓ_q) Regularization

- We can generalize to ℓ_q : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.



- Note: $\|w\|_q$ is only a norm if $q \geqslant 1$, but not for $q \in (0, 1)$
- When $q < 1$, the ℓ_q constraint is non-convex, so it is hard to optimize; lasso is good enough in practice
- ℓ_0 $(\|w\|_0)$ is defined as the number of non-zero weights, i.e. subset selection

Minimizing the lasso objective

Minimizing the lasso objective

- The ridge regression objective is differentiable (and there is a closed form solution)
- Lasso objective function:

$$\min_{w \in \mathbf{R}^d} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda \|w\|_1$$

- $\|w\|_1 = |w_1| + \ldots + |w_d|$ is not differentiable!

Minimizing the lasso objective

- The ridge regression objective is differentiable (and there is a closed form solution)
- Lasso objective function:

$$\min_{w \in \mathbf{R}^d} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda \|w\|_1$$

- $\|w\|_1 = |w_1| + \ldots + |w_d|$ is not differentiable!
- We will briefly review three approaches for finding the minimum:
  - Quadratic programming
  - Projected SGD
  - Coordinate descent

Rewriting the Absolute Value

- Consider any number $a \in \mathrm{R}$.
- Let the **positive part** of a be
$$a^{+} = a1(a \geqslant 0).$$
- Let the **negative part** of a be
$$a^{-} = -a1(a \leqslant 0).$$

Rewriting the Absolute Value

- Consider any number $a \in \mathbf{R}$.
- Let the **positive part** of a be
$$a^+ = a \mathbb{1}(a \geqslant 0).$$
- Let the **negative part** of a be
$$a^- = -a \mathbb{1}(a \leqslant 0).$$
- Is it always the case that $a^+ \geqslant 0$ and $a^- \geqslant 0$?

Rewriting the Absolute Value

- Consider any number $a \in R$.
- Let the **positive part** of a be
$$a^+ = a1(a \geqslant 0).$$
- Let the **negative part** of a be
$$a^- = -a1(a \leqslant 0).$$
- Is it always the case that $a^+ \geqslant 0$ and $a^- \geqslant 0$?
- How do you write a in terms of a^+ and a^-?

Rewriting the Absolute Value

- Consider any number $a \in R$.
- Let the **positive part** of a be
$$a^{+} = a1(a \geqslant 0).$$
- Let the **negative part** of a be
$$a^{-} = -a1(a \leqslant 0).$$
- Is it always the case that $a^{+} \geqslant 0$ and $a^{-} \geqslant 0$?
- How do you write a in terms of a^{+} and a^{-}?
- How do you write $|a|$ in terms of a^{+} and a^{-}?

The Lasso as a Quadratic Program

Substituting $w = w^+ - w^-$ and $|w| = w^+ + w^-$ results in an equivalent problem:

$$\min_{w^+,w^-} \quad \sum_{i=1}^{n} \left(\left(w^+ - w^-\right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^-\right)$$

$$\text{subject to} \quad w_i^+ \geqslant 0 \text{ for all } i \quad \text{and} \quad w_i^- \geqslant 0 \text{ for all } i,$$

- This objective is **differentiable** (in fact, **convex and quadratic**)
- How many variables does the new objective have?
- This is a **quadratic program**: a convex quadratic objective with linear constraints.
- Quadratic programming is a very well understood problem; we can plug this into a generic QP solver.

Are we missing some constraints?

We have claimed that the following objective is equivalent to the lasso problem:

$$\begin{array}{ll} \min_{w^+, w^-} & \sum_{i=1}^{n} \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^- \right) \\ \text{subject to} & w_i^+ \geqslant 0 \text{ for all } i \qquad w_i^- \geqslant 0 \text{ for all } i, \end{array}$$

- When we plug this optimization problem into a QP solver,
  - it just sees $2d$ variables and $2d$ constraints.
  - Doesn't know we want w_i^+ and w_i^- to be positive and negative parts of w_i.
- Turns out that these constraints will be satisfied anyway!
- To make it clear that the solver isn't aware of the constraints of w_i^+ and w_i^-, let's denote them a_i and b_i

(Trivially) reformulating the lasso problem:

$$
\begin{aligned}
\min_{w} \min_{a,b} \quad & \sum_{i=1}^{n} \left((a-b)^T x_i - y_i \right)^2 + \lambda 1^T (a+b) \\
\text{subject to} \quad & a_i \geqslant 0 \text{ for all } i \qquad b_i \geqslant 0 \text{ for all } i, \\
& a - b = w \\
& a + b = |w|
\end{aligned}
$$

The Lasso as a Quadratic Program

(Trivially) reformulating the lasso problem:

$$\begin{aligned}
\min_{w}\ \min_{a,b} \quad & \sum_{i=1}^{n}\left((a-b)^T x_i - y_i\right)^2 + \lambda 1^T(a+b) \\
\text{subject to} \quad & a_i \geqslant 0 \text{ for all } i \qquad b_i \geqslant 0 \text{ for all } i, \\
& a - b = w \\
& a + b = |w|
\end{aligned}$$

Claim: Don't need the constraint $a+b=|w|$.

Exercise: Prove by showing that the optimal solutions a^* and b^* satisfies $\min(a^*, b^*) = 0$, hence $a^* + b^* = |w|$.

The Lasso as a Quadratic Program

$$\begin{aligned}
\min_{w} \min_{a,b} \quad & \sum_{i=1}^{n} \left((a-b)^T x_i - y_i \right)^2 + \lambda 1^T (a+b) \\
\text{subject to} \quad & a_i \geqslant 0 \text{ for all } i \qquad b_i \geqslant 0 \text{ for all } i, \\
& a - b = w
\end{aligned}$$

Claim: Can remove $\min_w$ and the constraint $a-b=w$.

Exercise: Prove by switching the order of the minimization.

Projected SGD

- Now that we have a differentiable objective, we could also use gradient descent
- But how do we handle the constraints?

$$
\begin{aligned}
\min_{w^+, w^- \in \mathbf{R}^d} & \sum_{i=1}^{n} \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^- \right) \\
\text{subject to } & w_i^+ \geqslant 0 \text{ for all } i \\
& w_i^- \geqslant 0 \text{ for all } i
\end{aligned}
$$

- Projected SGD is just like SGD, but after each step
  - We project w^+ and w^- into the constraint set.
  - In other words, if any component of w^+ or w^- becomes negative, we set it back to 0.

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \ldots, w_d)$ over $w = (w_1, \ldots, w_d) \in \mathbb{R}^d$.

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \ldots, w_d)$ over $w = (w_1, \ldots, w_d) \in \mathbf{R}^d$.

- In gradient descent or SGD, each step potentially changes all entries of w.

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \ldots, w_d)$ over $w = (w_1, \ldots, w_d) \in \mathrm{R}^d$.

- In gradient descent or SGD, each step potentially changes all entries of w.
- In **coordinate descent**, each step adjusts only a single coordinate w_i.

$$w_i^{\text{new}} = \underset{w_i}{\arg\min}\, L(w_1, \ldots, w_{i-1}, \mathrm{w_i}, w_{i+1}, \ldots, w_d)$$

- Solving the argmin for a particular coordinate may itself be an iterative process.
- Coordinate descent is an effective method when it's easy (or easier) to minimize w.r.t. one coordinate at a time

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \ldots w_d)$ over $w = (w_1, \ldots, w_d) \in \mathrm{R}^d$.

- **Initialize** $w^{(0)} = 0$
- **while** not converged:
  - Choose a coordinate $j \in \{1, \ldots, d\}$
  - $w_j^{\text{new}} \leftarrow \arg\min_{w_j} L(w_1^{(t)}, \ldots, w_{j-1}^{(t)}, \mathrm{w_j}, w_{j+1}^{(t)}, \ldots, w_d^{(t)})$
  - $w_j^{(t+1)} \leftarrow w_j^{\text{new}}$ and $w^{(t+1)} \leftarrow w^{(t)}$
  - $t \leftarrow t + 1$

- Random coordinate choice $\implies$ **stochastic coordinate descent**
- Cyclic coordinate choice $\implies$ **cyclic coordinate descent**

Coordinate Descent Method for Lasso

The lasso objective coordinate minimization has a closed form! If

$$\hat{w}_j = \arg\min_{w_j \in \mathrm{R}} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda |w|_1$$

Then

$$\hat{w}_j = \begin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \\ 0 & \text{if } c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

$$a_j = 2\sum_{i=1}^{n} x_{i,j}^2 \qquad c_j = 2\sum_{i=1}^{n} x_{i,j}(y_i - w_{-j}^T x_{i,-j})$$

where w_{-j} is w without the j-th component, and $x_{i,-j}$ is x_i without the j-th component.

Coordinate Descent in General

- In general, coordinate descent is not competitive with gradient descent: its convergence rate is slower and the iteration cost is similar

Coordinate Descent in General

- In general, coordinate descent is not competitive with gradient descent: its convergence rate is slower and the iteration cost is similar
- But it works very well for certain problems

Coordinate Descent in General

- In general, coordinate descent is not competitive with gradient descent: its convergence rate is slower and the iteration cost is similar
- But it works very well for certain problems
- Very simple and easy to implement

Coordinate Descent in General

- In general, coordinate descent is not competitive with gradient descent: its convergence rate is slower and the iteration cost is similar
- But it works very well for certain problems
- Very simple and easy to implement
- Example applications: lasso regression, SVMs