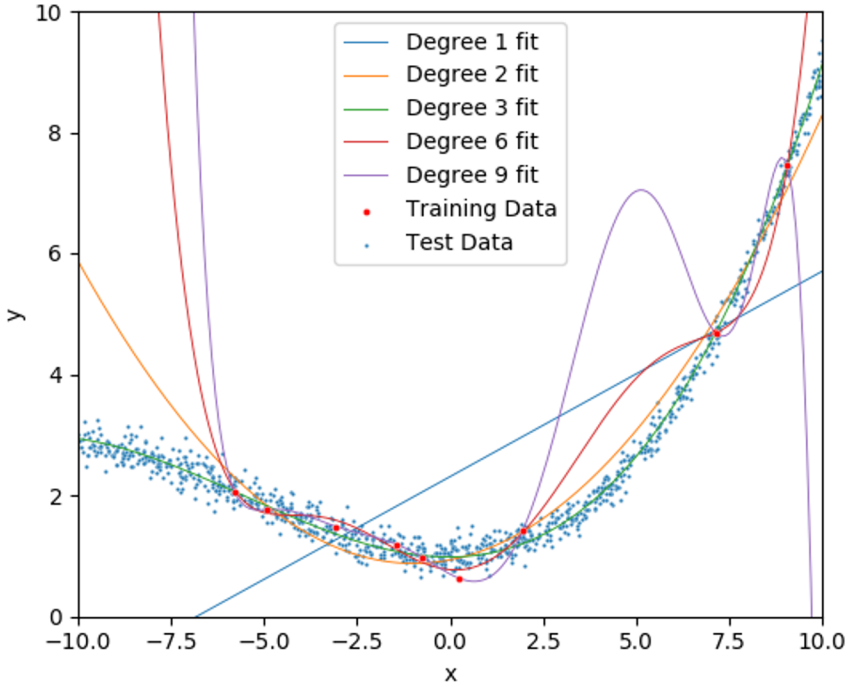
LECTURE 16

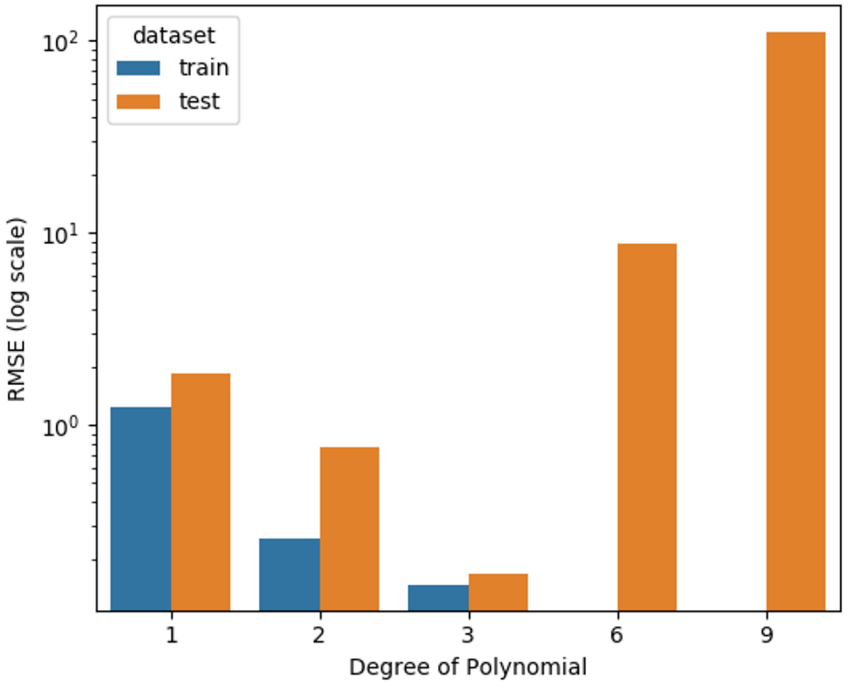
Cross-Validation and Regularization

Different methods for ensuring the generalizability of our models to unseen data.

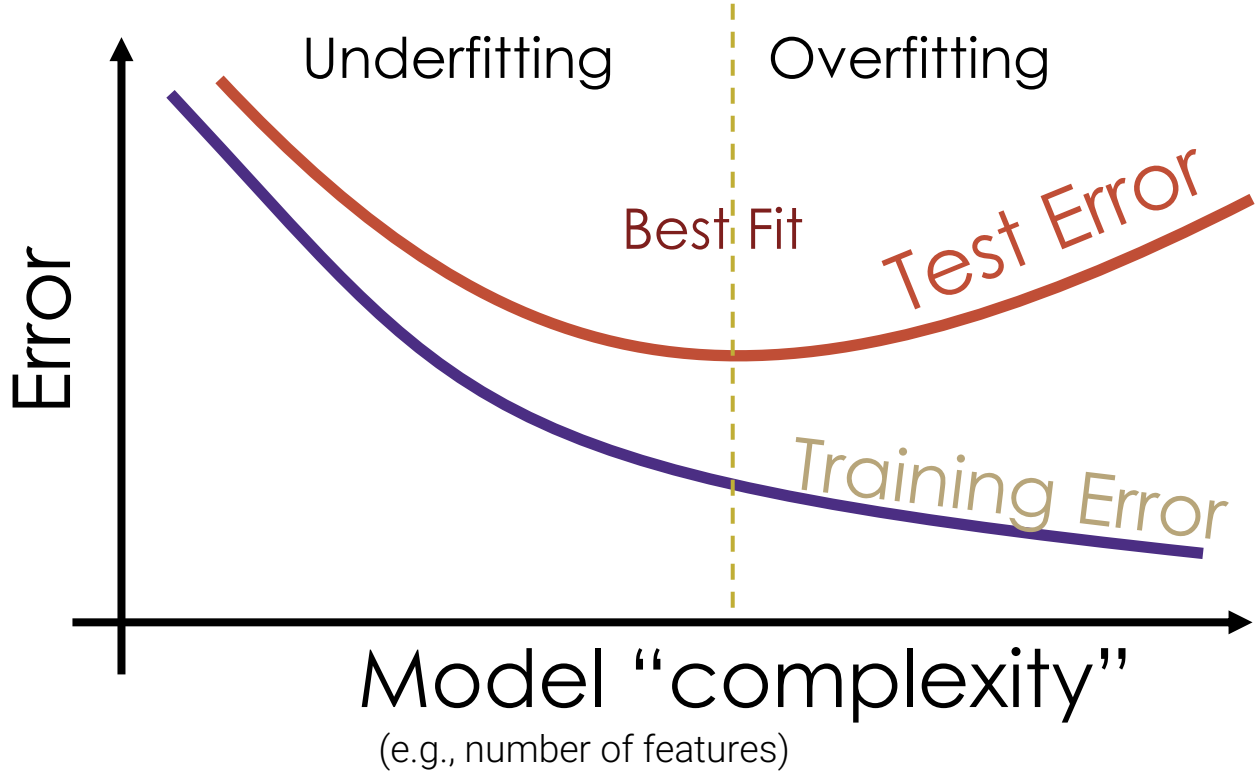
Cross-Validation

Training Error vs Test Error





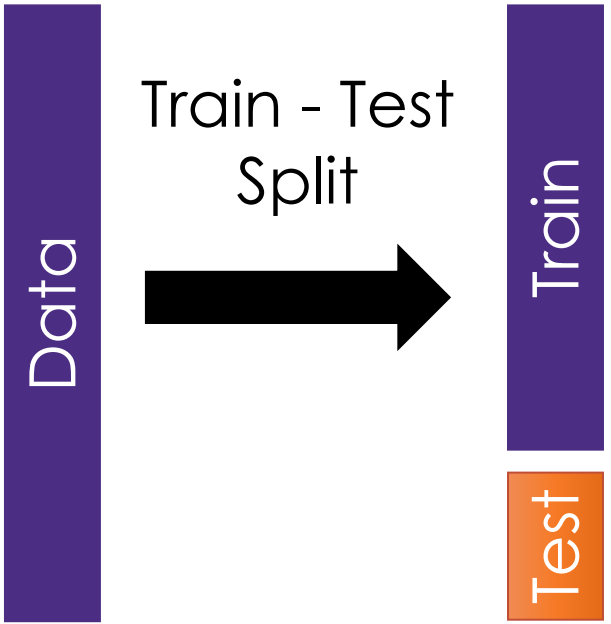
Training Error vs Test Error



Training error typically *underestimates* **test error**.

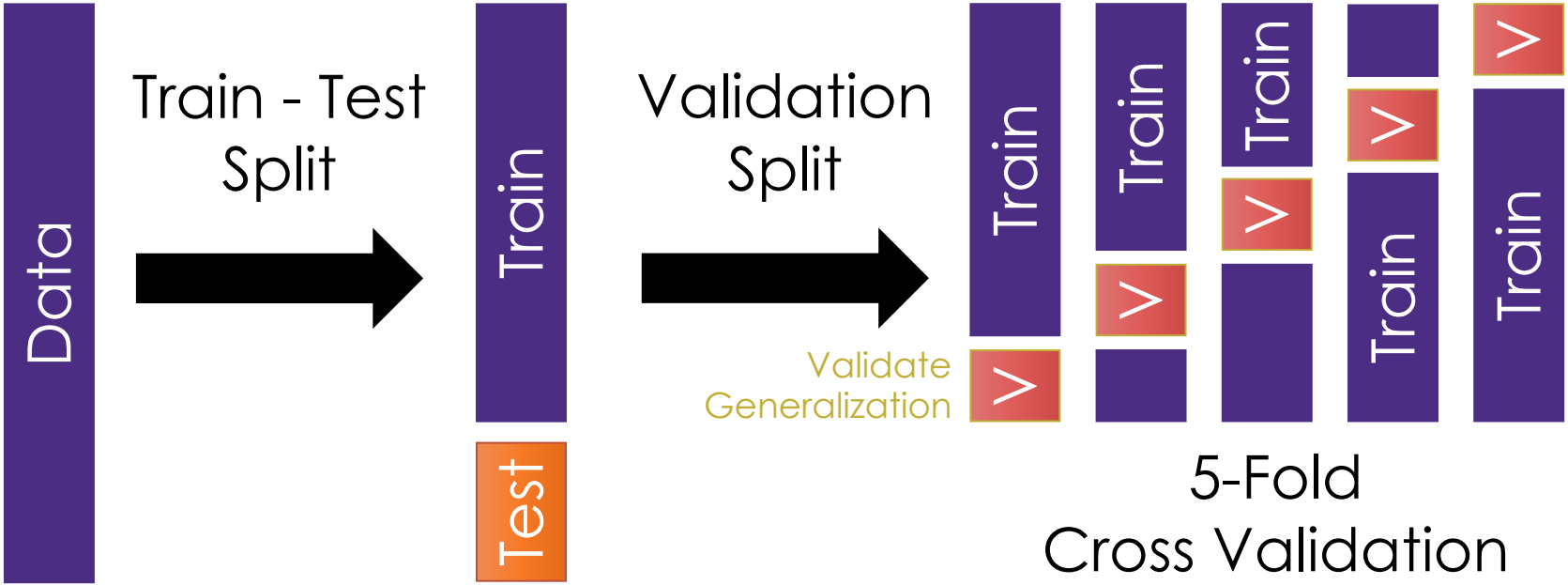
Generalization: *The Train-Test Split*

- **Training Data:** used to fit model
- **Test Data:** check generalization error
- How to split?
  - Randomly, Temporally, Geo…
  - Depends on application (usually randomly)
- What size? (90%-10%)
  - Larger training set – more complex models
  - Larger test set – better estimate of generalization error
  - Typically between 75%-25% and 90%-10%



You can only use the test dataset once after deciding on the model.

Generalization: *Validation Split*



Cross validation ***simulates multiple train test-splits*** *within the training data.*

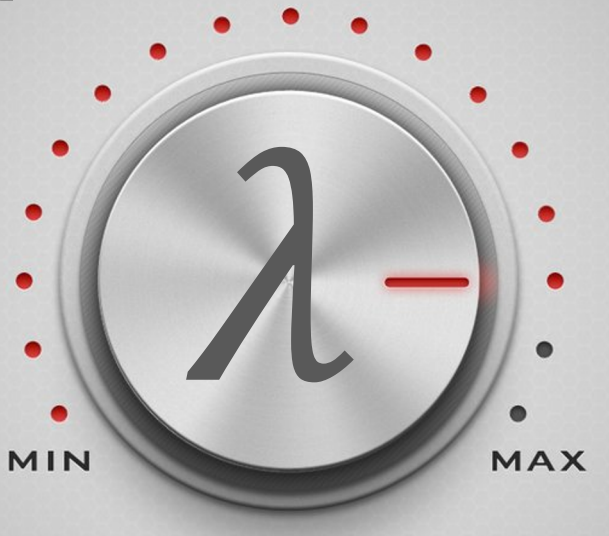
Recipe for Successful Generalization

1. Split your data into **training** and **test** sets (90%, 10%)
2. Use **only the training data** when designing, training, and tuning the model
    - Use **cross validation** to test *generalization* during this phase
    - **Do not look at the test data!**
1. Commit to your final model and train once more using **only the training data.**
2. Test the final model using the **test data**.
3. Train on **all available data** and ship it!

Demo

Regularization

Controlling the
Model Complexity



Basic Idea

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that:

f_θ does not “overfit”

Can we make this more formal?

Basic Idea

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that:

$$\text{Complexity}(f_\theta) \leq \beta$$

Regularization Hyperparameter

How do we define this?

Idealized Notion of Complexity

$$\text{Complexity}(f_\theta) \leq \beta$$

- Focus on complexity of **linear models**:
  - Number and kinds of features
- Ideal definition:

$$\mathbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right]$$

Number of non-zero parameters

- Why?

Ideal “Regularization”

Find the best value of θ which uses fewer than β features.

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \textbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

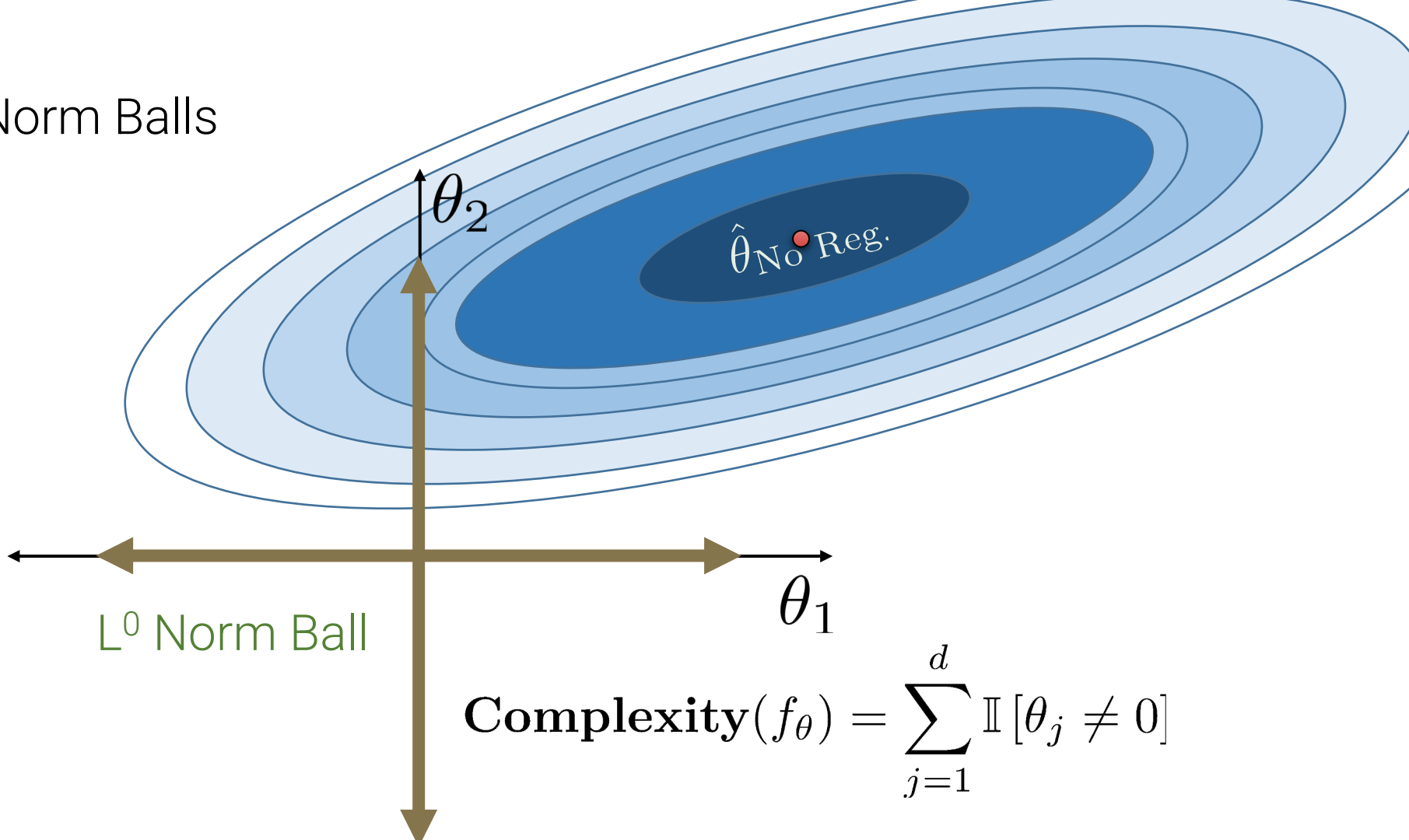
Such that:

Need an approximation!

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right] \leq \beta$$

Combinatorial search problem – NP-hard to solve in general.

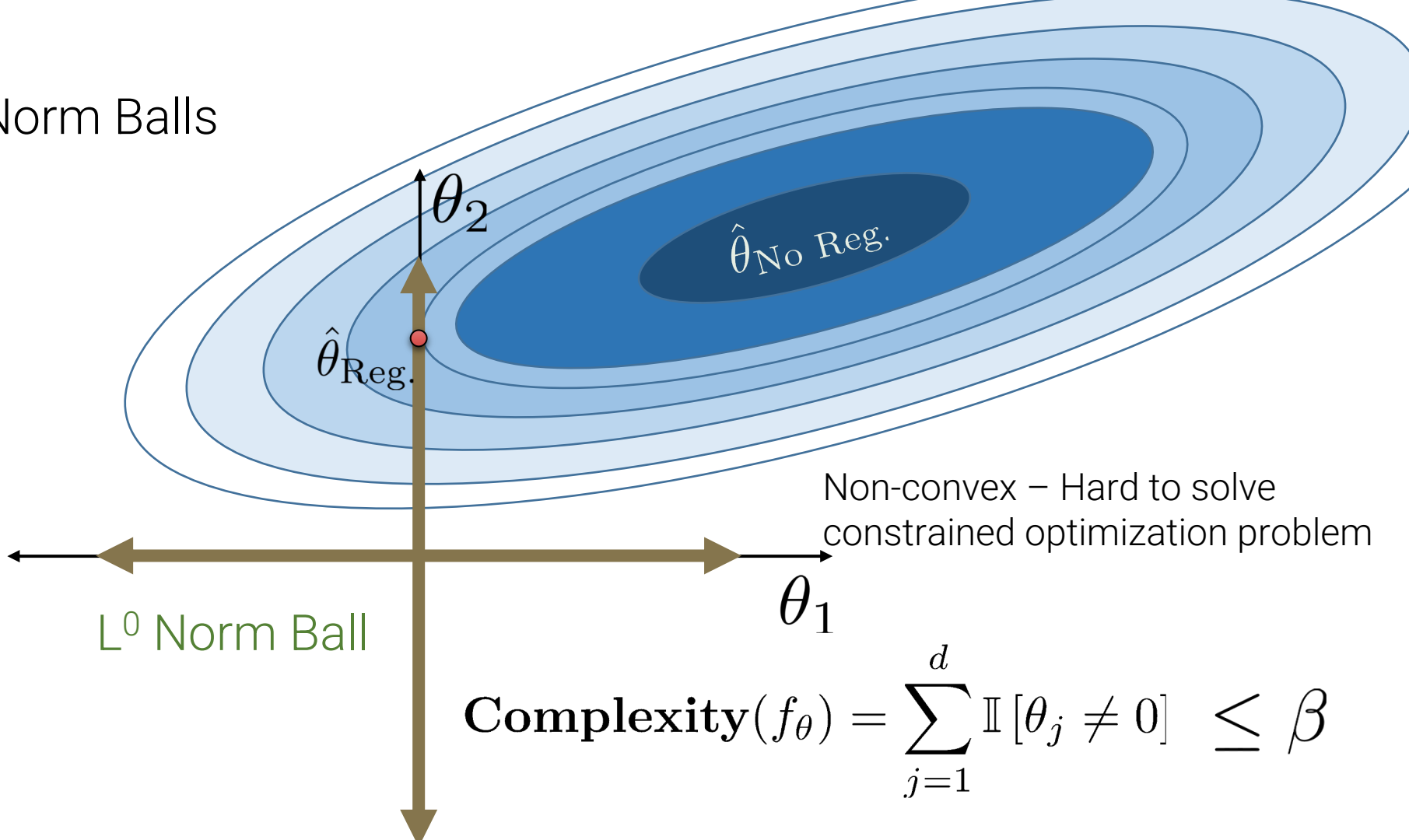
Norm Balls



L^0 Norm Ball

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right]$$

Norm Balls

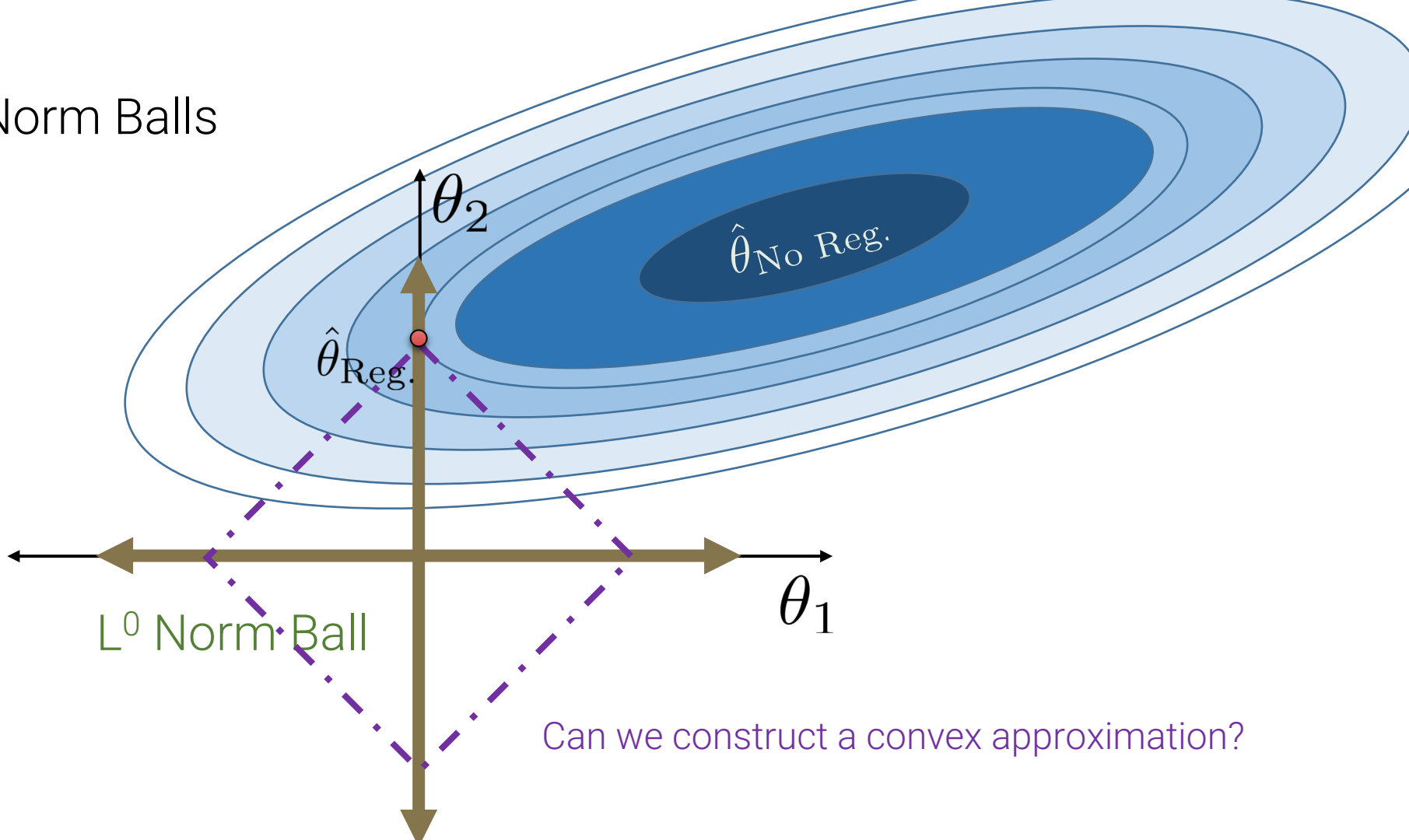


Non-convex – Hard to solve constrained optimization problem

L^0 Norm Ball

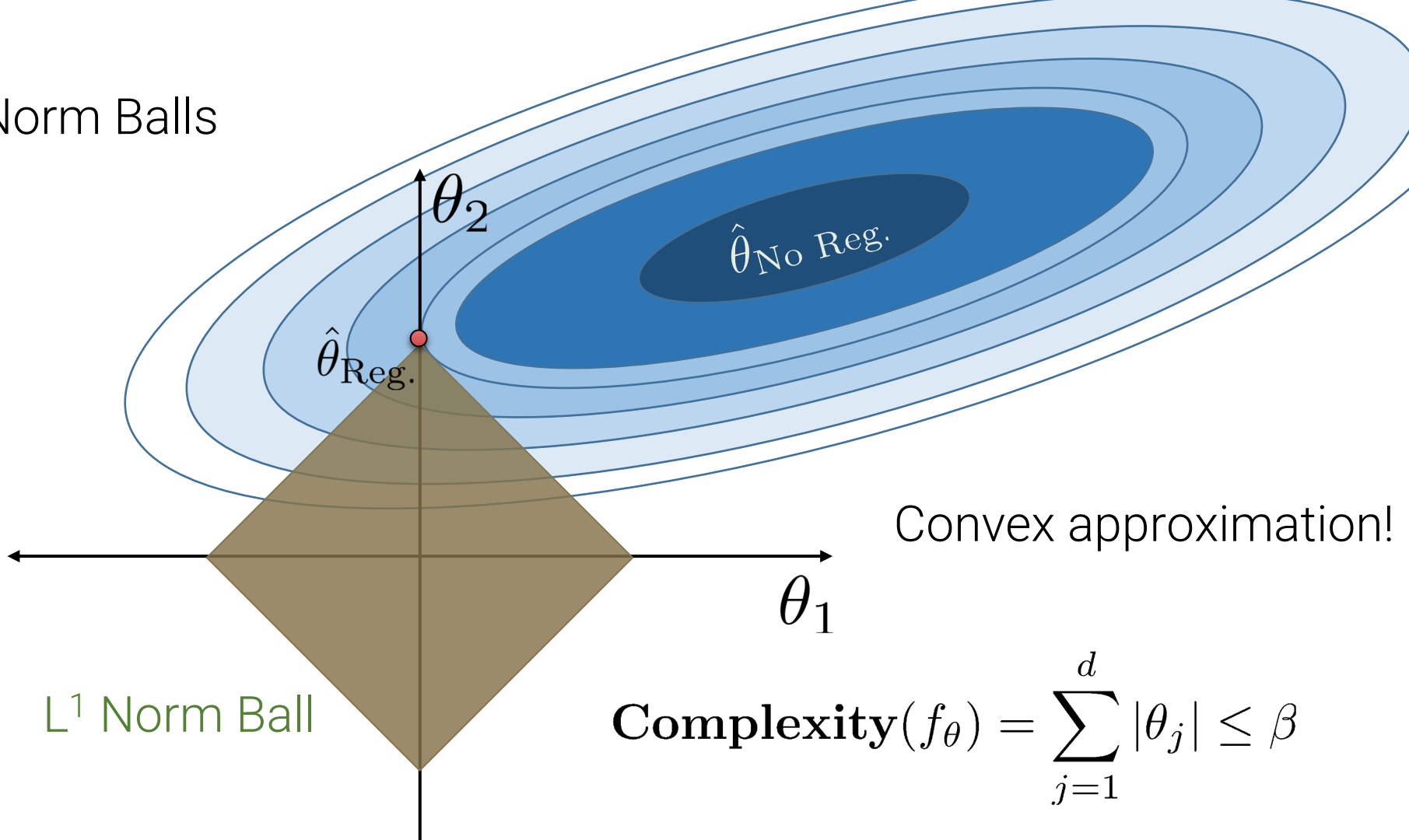
$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right] \leq \beta$$

Norm Balls



Can we construct a convex approximation?

Norm Balls

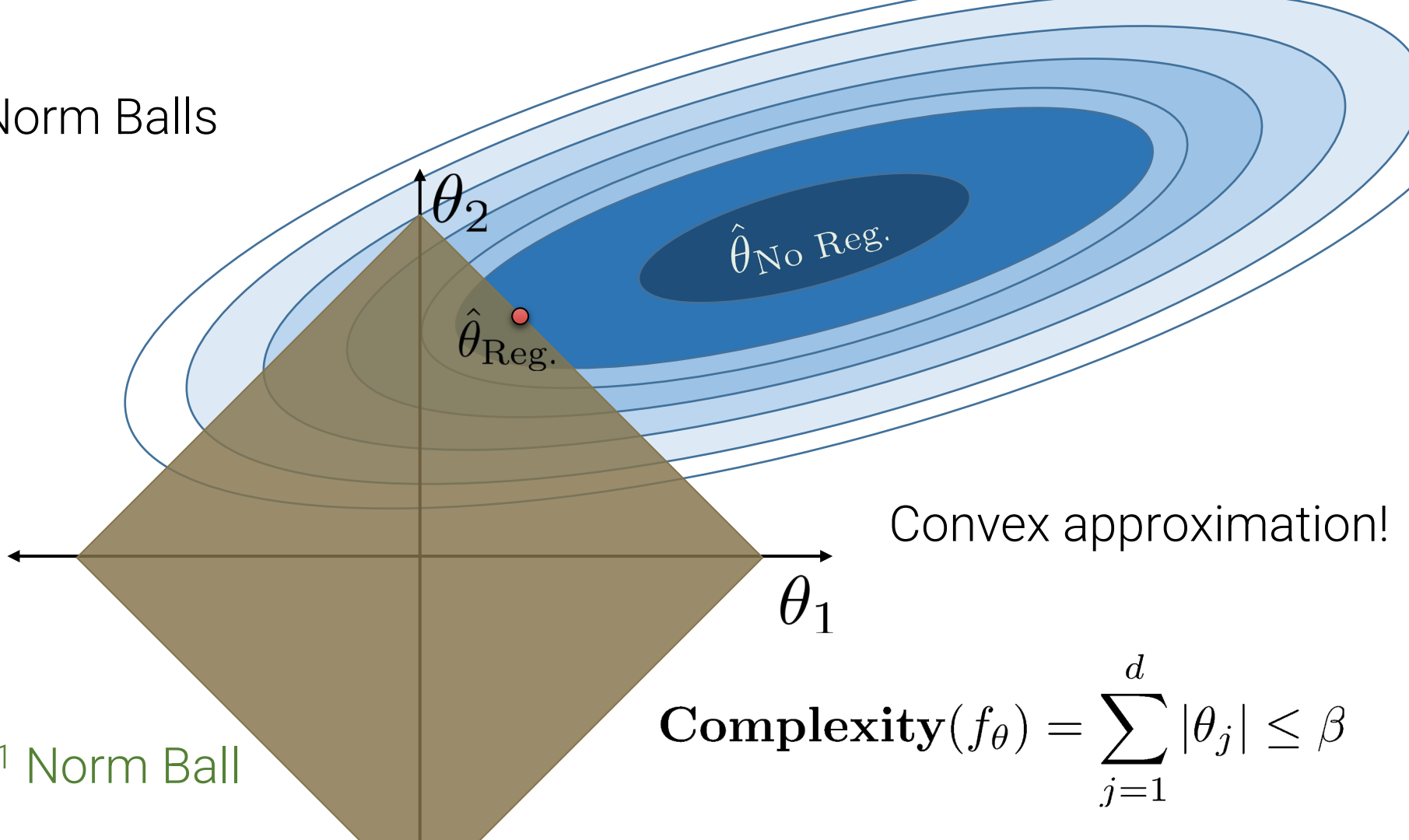


Convex approximation!

L^1 Norm Ball

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$$

Norm Balls

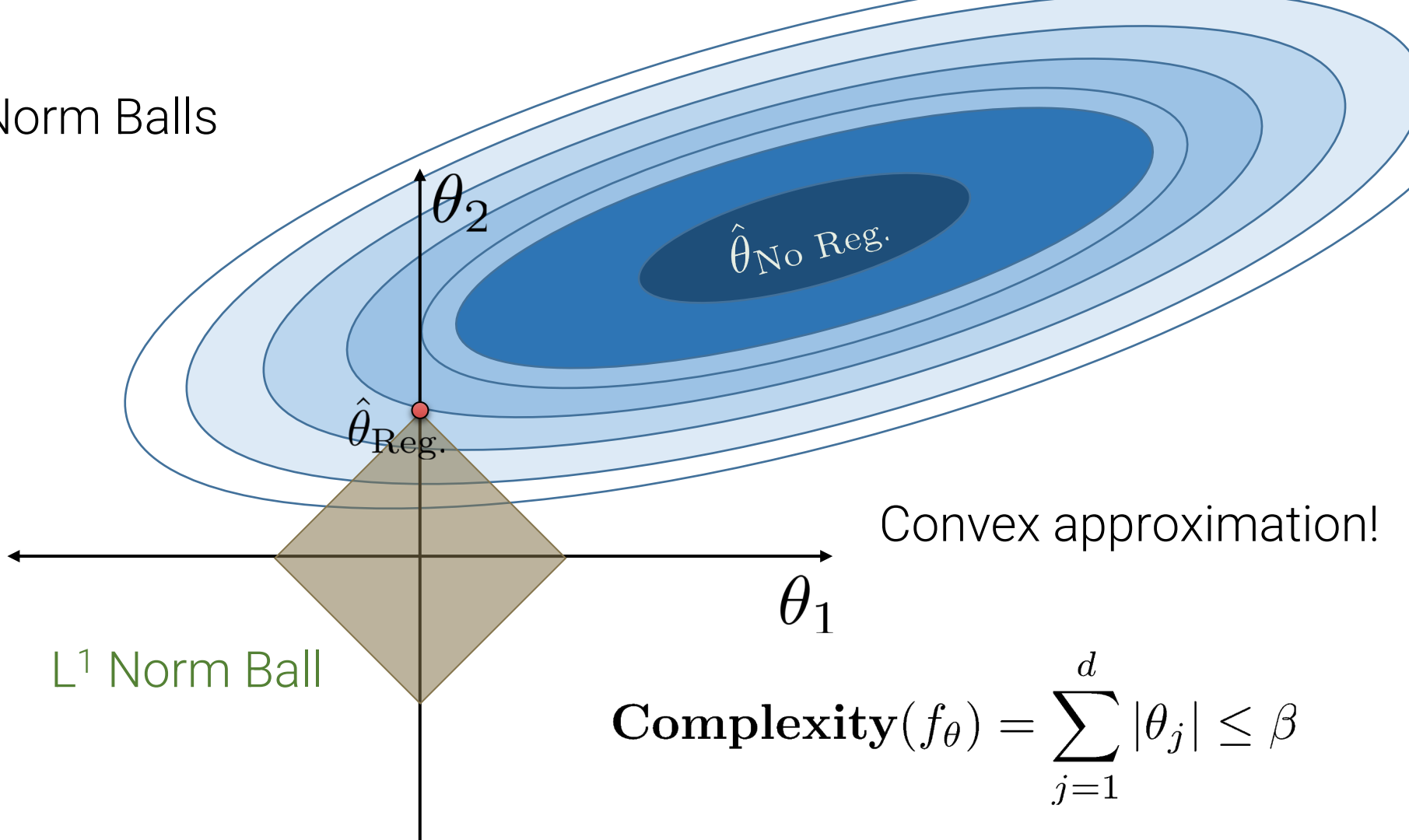


Convex approximation!

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$$

L^1 Norm Ball

Norm Balls

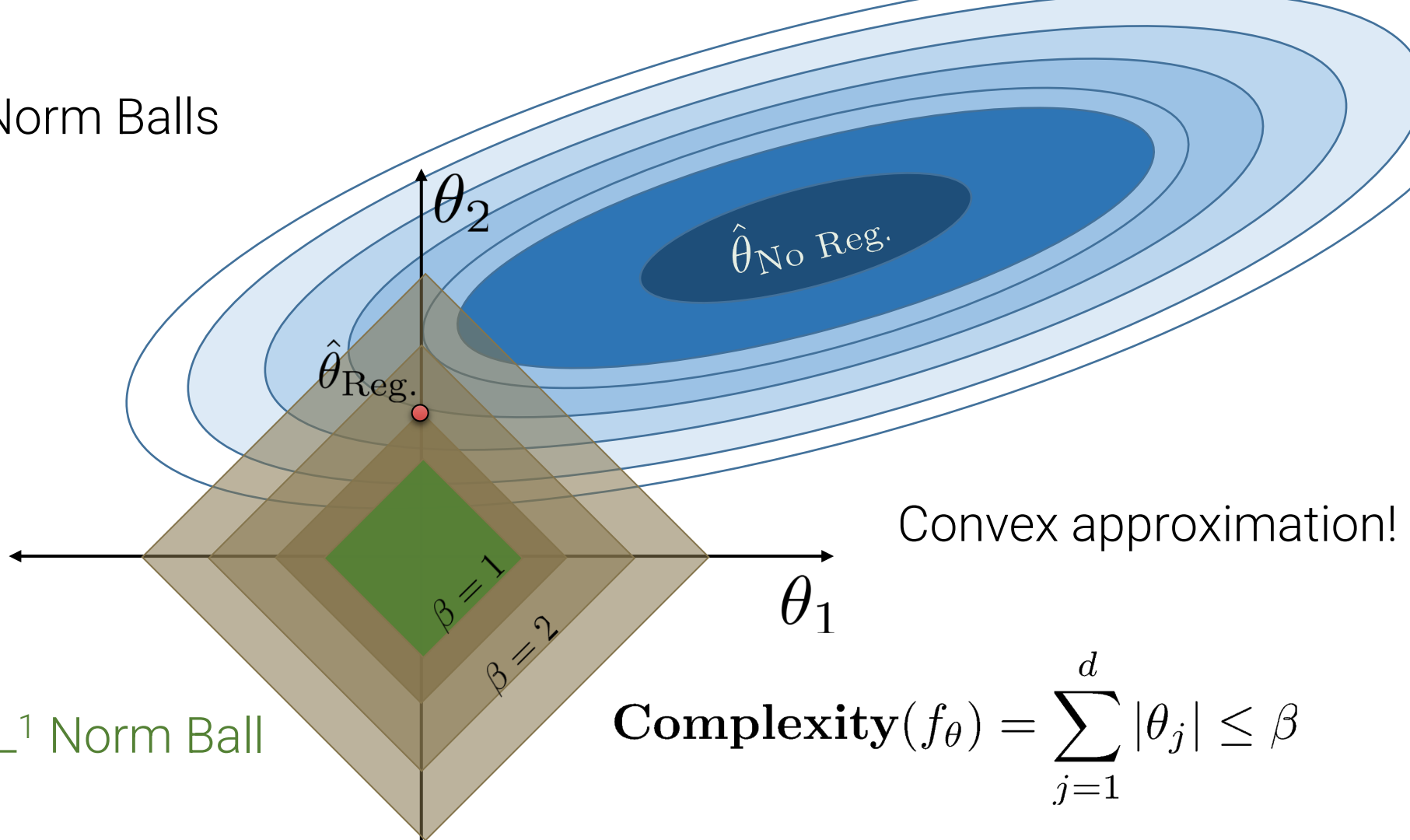


Convex approximation!

L^1 Norm Ball

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$$

Norm Balls

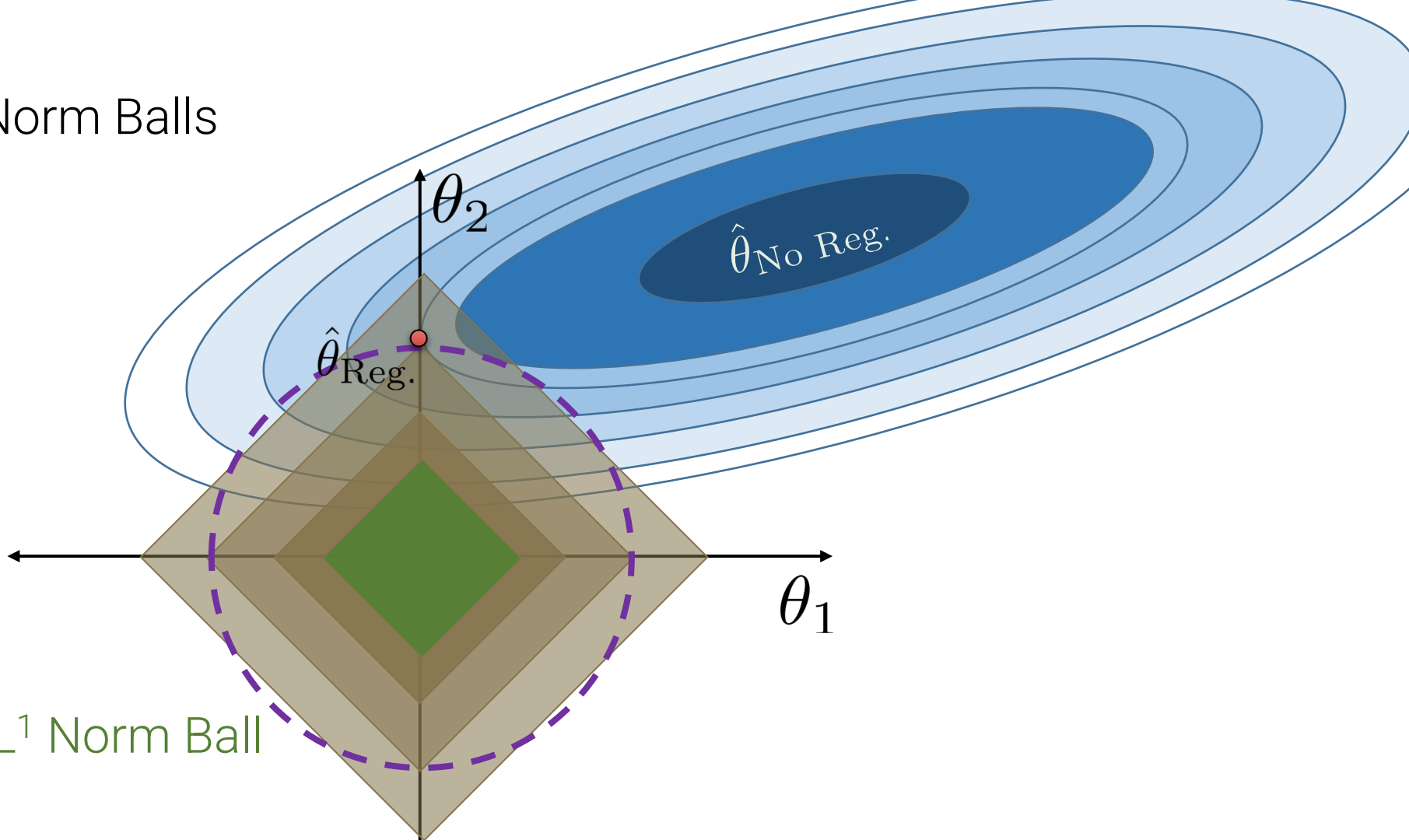


Convex approximation!

L^1 Norm Ball

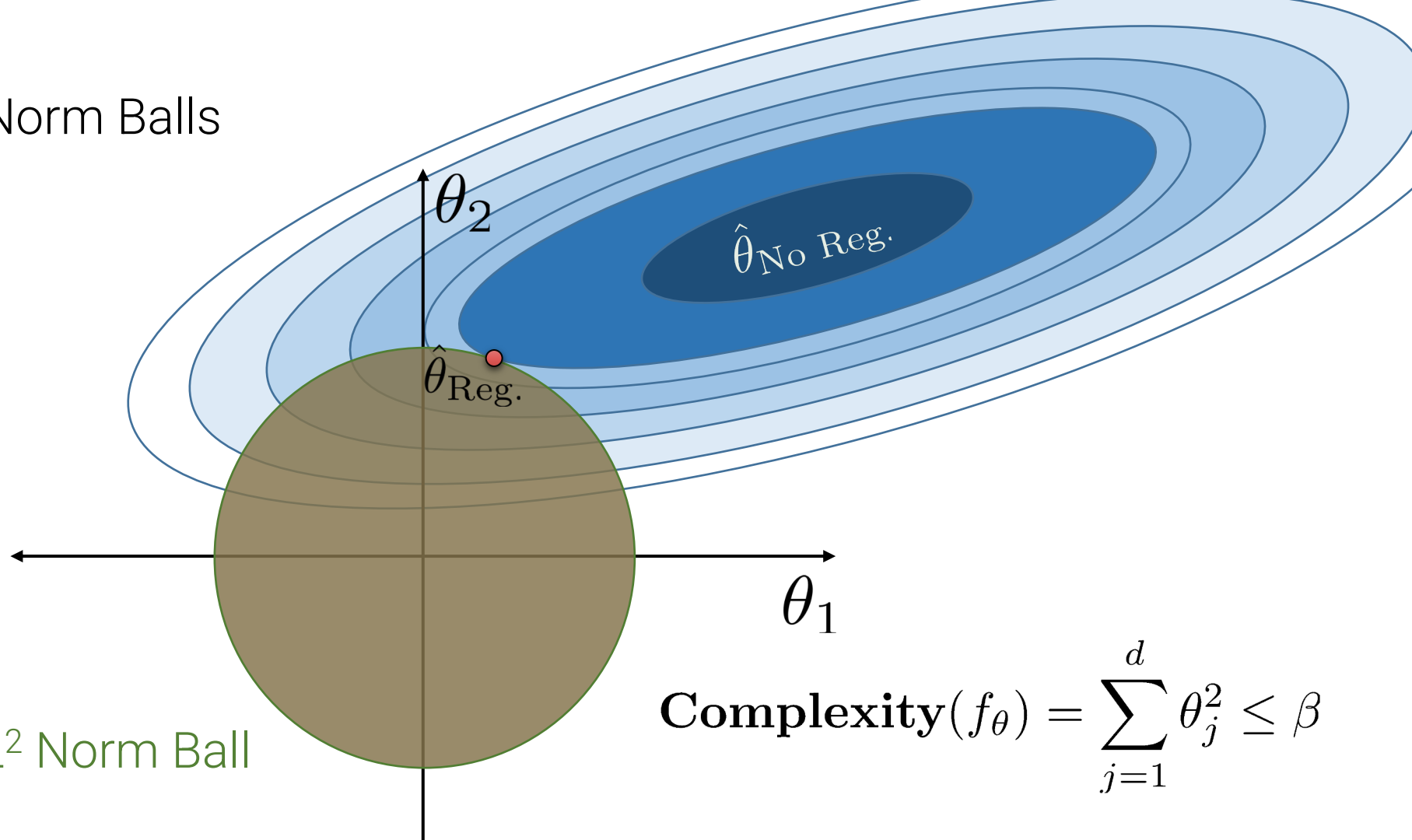
$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$$

Norm Balls



L^1 Norm Ball

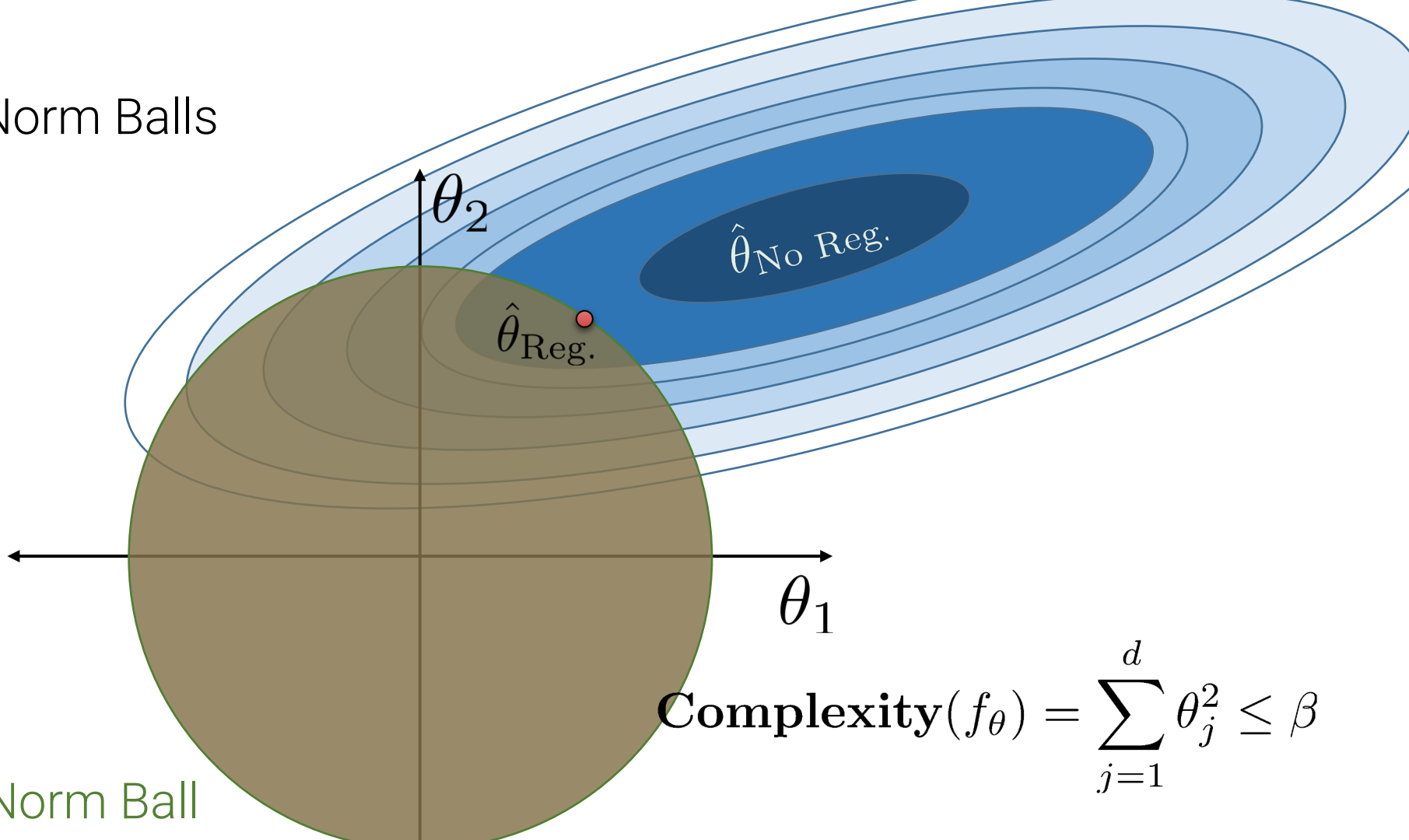
Norm Balls



$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \theta_j^2 \leq \beta$$

L^2 Norm Ball

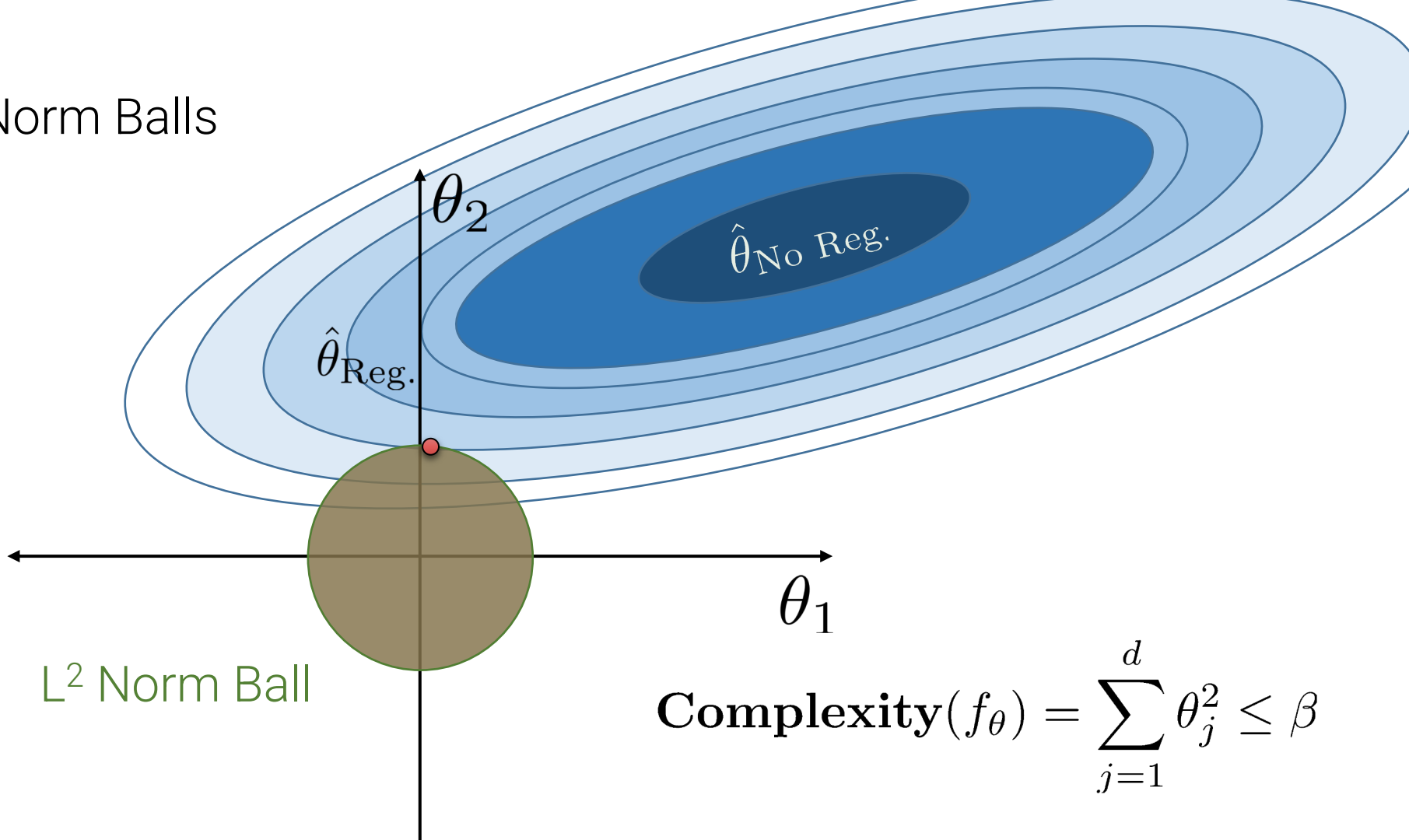
Norm Balls



$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \theta_j^2 \leq \beta$$

L^2 Norm Ball

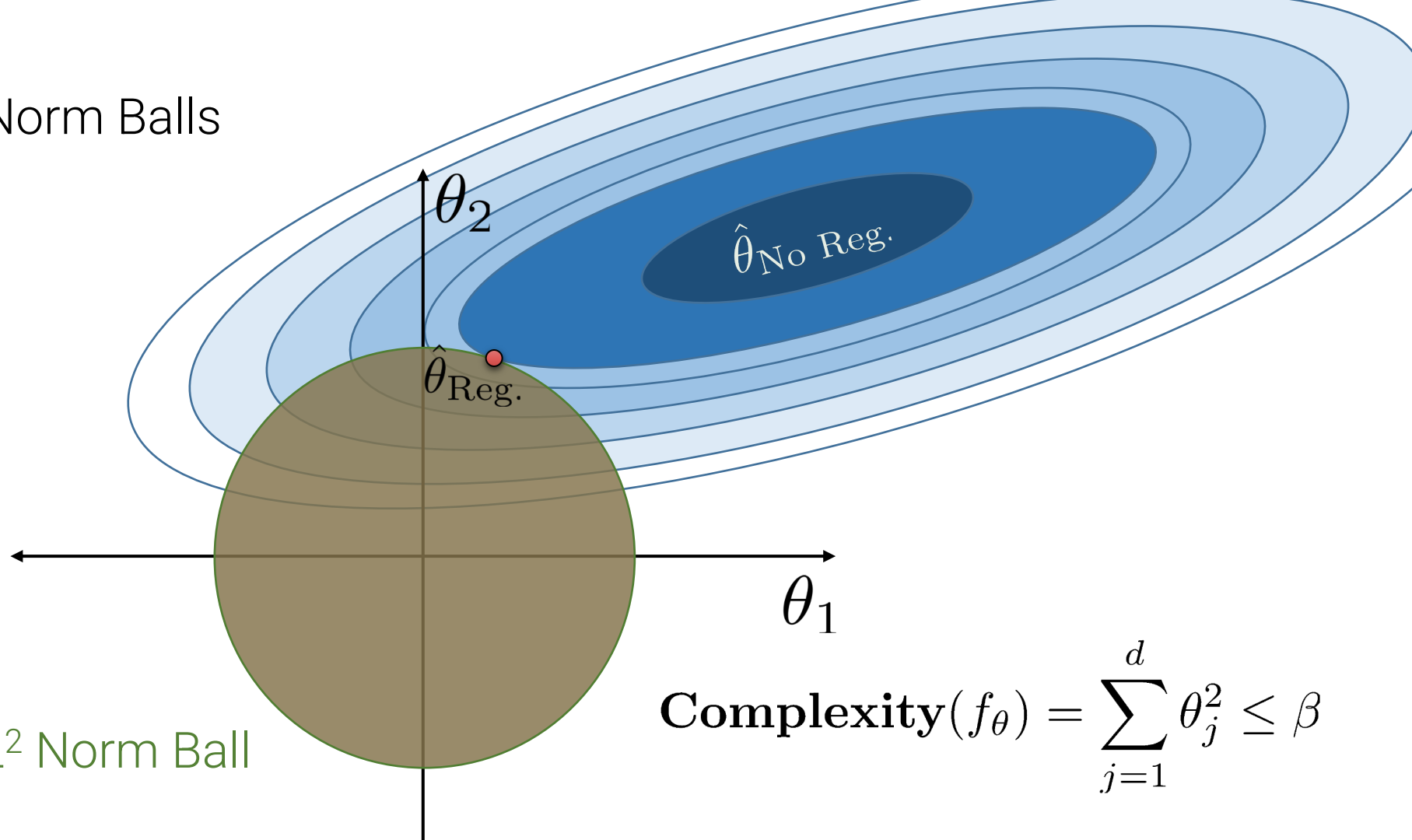
Norm Balls



L^2 Norm Ball

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \theta_j^2 \leq \beta$$

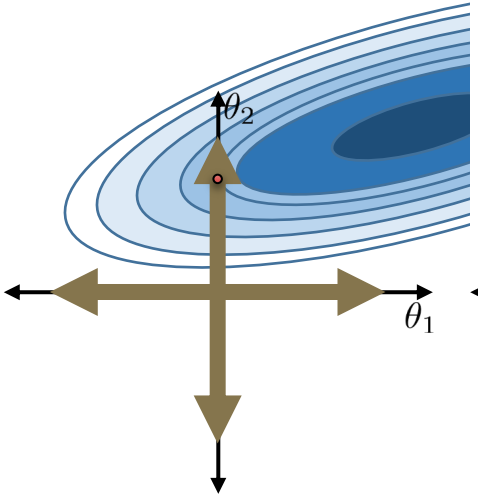
Norm Balls



$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \theta_j^2 \leq \beta$$

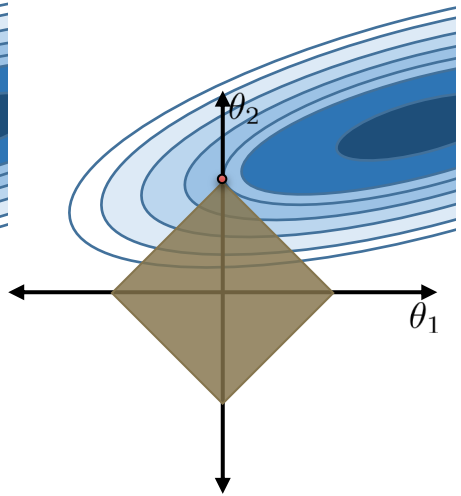
L^2 Norm Ball

L^0 Norm Ball



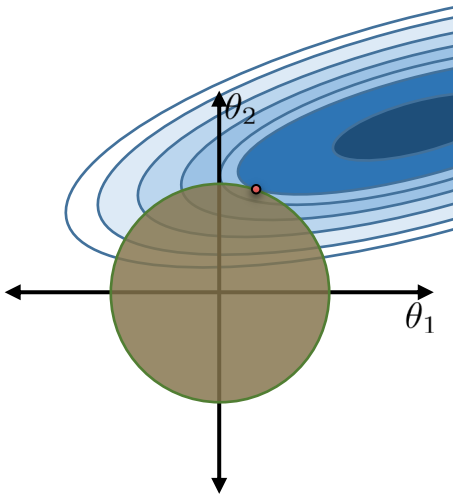
Ideal for
Feature Selection
but combinatorically
difficult to optimize

L^1 Norm Ball



Encourages
sparse solutions
Convex!

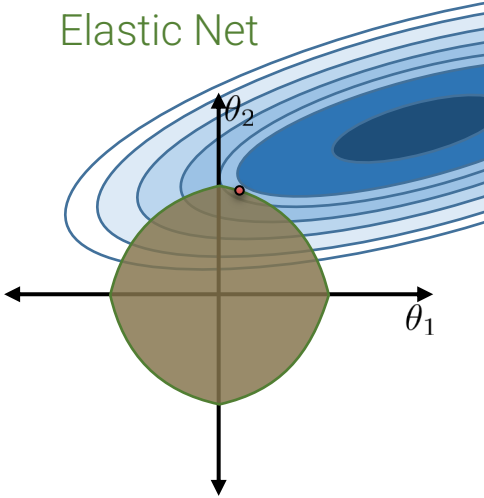
L^2 Norm Ball



Spreads weight
over features **(robust)**,
but does not
encourage sparsity

$L^1 + L^2$ Norm

Elastic Net



Compromise
Need to tune
two regularization
hyperparameters

Reformulating the Problem

Generic Regularization (Constrained)

Defining $\mathbf{Complexity}(f_\theta) = R(\theta)$

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that: $R(\theta) \leq \beta$

There is an equivalent unconstrained formulation (obtained by Lagrangian duality)

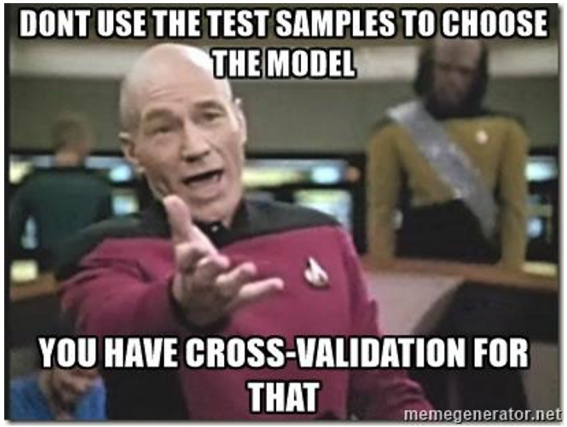
Generic Regularization (Unconstrained)

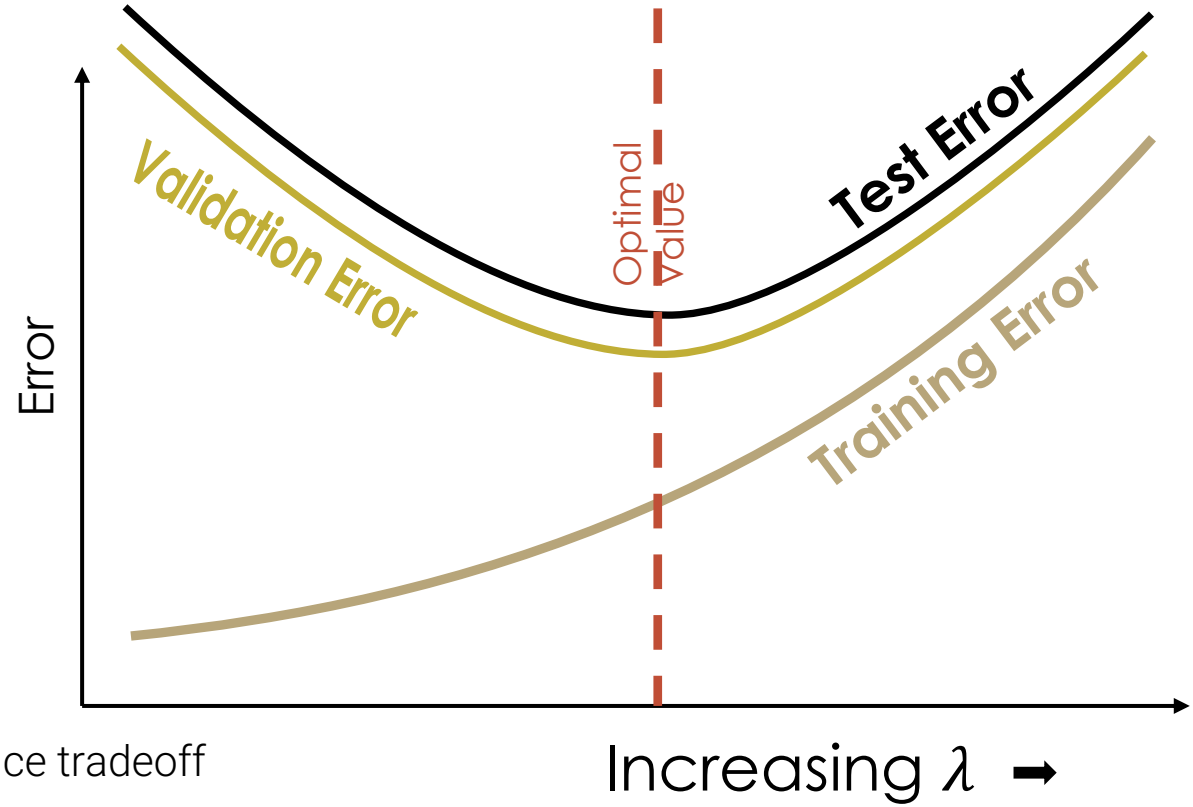
Defining $\mathbf{Complexity}(f_\theta) = R(\theta)$

$$\hat{\theta} = \arg\min_{\theta} \left[\left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right) \right) + \lambda R(\theta) \right]$$

Regularization Hyperparameter

Determining the Optimal λ





Value of λ determines bias-variance tradeoff

Optimal λ determined through cross validation

Standardization and the Intercept Term

- `Height =` θ_1 `age_in_seconds +` θ_2 `weight_in_tons`

Small

Large

- Regularization penalized dimensions equally
- Standardization
  - Ensure that each dimensions has the same scale
  - centered around zero
- Intercept Terms
  - Typically don't regularize intercept term

Standardization

For each dimension *k*:

$$z_k = \frac{x_k - \mu_k}{\sigma_k}$$

Ridge and LASSO Regression

Ridge Regression

“Ridge Regression” is a term for the following specific combination of model, loss, and regularization:

- Model: $\hat{\mathbb{Y}} = \mathbb{X}\hat{\theta}$
- Loss: Squared loss
- Regularization: L2 regularization

The **objective function** we minimize for Ridge Regression is average squared loss, plus an added penalty:

$$\hat{\theta}_{\text{ridge}} = \arg\min_{\theta} \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda \sum_{j=1}^{d} \theta_i^2$$

Ridge Regression

We can also express this objective slightly differently:

$$\hat{\theta}_{\text{ridge}} = \arg\min_{\theta} \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda \sum_{j=1}^{d} \theta_i^2$$

$$\hat{\theta}_{\text{ridge}} = \arg\min_{\theta} \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda||\theta||_2^2$$

L2 norm of θ (hence, L2 regularization)

The latter representation ignores the fact that we typically don't regularize the intercept term

Ridge Regression

Ridge Regression has a closed form solution, conveniently:

$$\hat{\theta}_{\mathbf{ridge}} = (\mathbb{X}^T\mathbb{X} + n\lambda I)^{-1}\mathbb{X}^T\mathbb{Y}$$

Identity matrix

Unlike OLS, there always exists a unique optimal parameter vector for Ridge Regression.
This is important, you should remember it!

LASSO Regression

“LASSO Regression” is a term for the following specific combination of model, loss, and regularization:

- Model: $\hat{\mathbb{Y}} = \mathbb{X}\hat{\theta}$
- Loss: Squared loss
- Regularization: L1 regularization

The **objective function** we minimize for LASSO Regression is average squared loss, plus an added penalty:

$$\hat{\theta}_{\text{LASSO}} = \arg\min_{\theta} \frac{1}{n} ||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda \sum_{j=1}^{d} |\theta_i|$$

LASSO Regression

We can also express this objective slightly differently:

$$\hat{\theta}_{\text{LASSO}} = \arg\min_{\theta} \frac{1}{n} ||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda \sum_{j=1}^{d} |\theta_i|$$

$$\hat{\theta}_{\text{LASSO}} = \arg\min_{\theta} \frac{1}{n} ||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda ||\theta||_1$$

Unfortunately, there is no closed-form solution for the optimal parameter vector for LASSO. We must use numerical methods (like gradient descent).

Summary of Regression Methods

Name	Model	Loss	Reg.	Objective	Solution
OLS	$\hat{\mathbb{Y}} = \mathbb{X}\hat{\theta}$	Squared loss	None	$\frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2$	$\hat{\theta}_{\text{OLS}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$
Ridge Regression	$\hat{\mathbb{Y}} = \mathbb{X}\hat{\theta}$	Squared loss	L2	$\frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2 + \lambda\sum_{j=1}^{d}\theta_i^2$	$\hat{\theta}_{\text{ridge}} = (\mathbb{X}^T\mathbb{X} + n\lambda I)^{-1}\mathbb{X}^T\mathbb{Y}$
LASSO	$\hat{\mathbb{Y}} = \mathbb{X}\hat{\theta}$	Squared loss	L1	$\frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2 + \lambda\sum_{j=1}^{d}\|\theta_i\|$	No closed form

Fitting vs. Evaluating

While we may use a regularized objective function to determine our model's parameters, we still look at **(root) mean squared error** to evaluate our model's performance.

$$\hat{\theta}_{\text{ridge}} = \arg\min_{\theta} \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2 + \lambda \sum_{j=1}^{d} \theta_i^2$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \mathbb{X}_i^T \hat{\theta}_{\text{ridge}})^2} = \sqrt{\frac{1}{n}||\mathbb{Y} - \mathbb{X}\hat{\theta}_{\text{ridge}}||_2^2}$$

The regularization penalty is there for the purposes of model fitting only.

Hyperparameters vs. Parameters

Parameters are facts about the world that we want to *estimate*

- Commonly denoted by p, θ, θ_i

Statistics are the *estimators* of the parameters, based on our data

- Commonly denoted by $\hat{p}, \hat{\theta}, \hat{\theta}_i$

Hyperparameters are design *choices* we make in our modeling process that affect our model, but do not directly come from the data

- examples: regularization hyperparameter, degree of polynomial
- Commonly denoted by λ, α, C

Demo