

INTRO to DATA SCIENCE

SESSION 4: REGRESSION & REGULARIZATION

Rob Hall

DAT13 SF // March 18, 2015

LAST TIME:

- INTRO TO ML**
- KNN CLASSIFICATION**
- INTRO TO MATPLOTLIB FOR VISUALIZATION**

QUESTIONS?

AGENDA

I. LINEAR REGRESSION (INCL. MULTIPLE REGRESSION)

II. POLYNOMIAL REGRESSION

III. REGULARIZATION

LAB:

**IV. IMPLEMENTING MULTIPLE REGRESSION & POLYNOMIAL
REGRESSION IN PYTHON**

- *Linear regression*
- *Multiple regression*
- *Polynomial regression*
- *The concept of minimizing some error or “cost” function*
- *Regularization*

I. LINEAR REGRESSION

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	???	???
<i>unsupervised</i>	???	???

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	<i>regression</i>	<i>classification</i>
<i>unsupervised</i>	<i>dimension reduction</i>	<i>clustering</i>

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*ε = **residual** (the prediction error)*

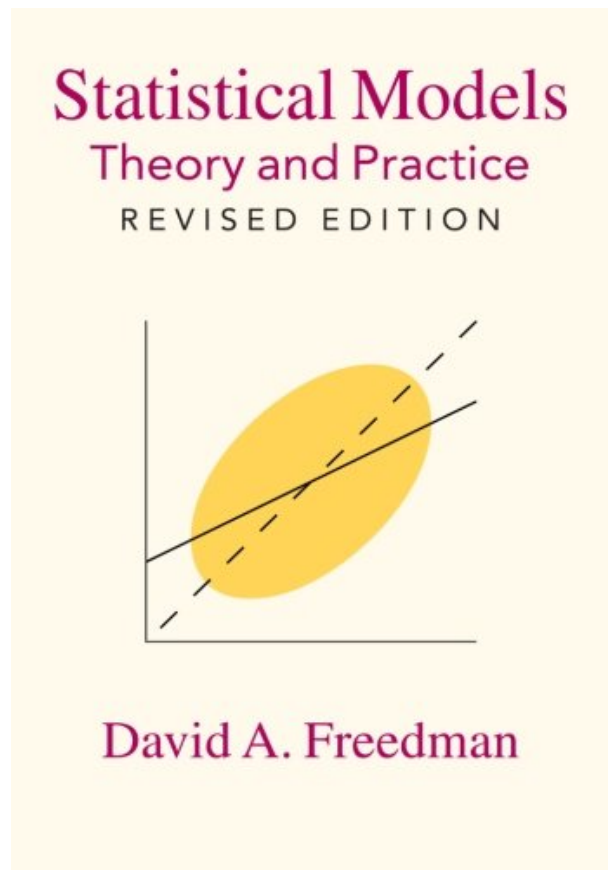
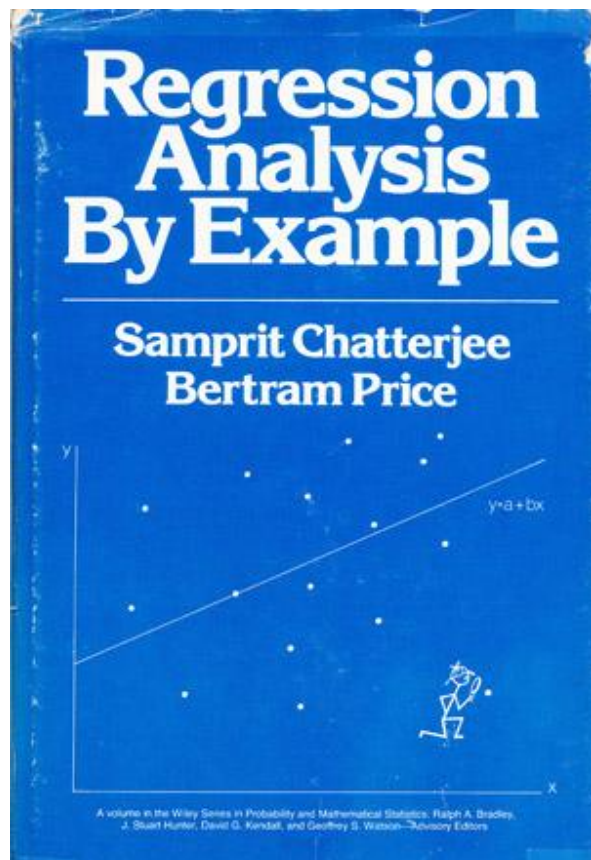
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$$y = \alpha + \beta_1 X_1 + \dots + \beta_n X_n + \varepsilon$$

Linear regression involves several technical assumptions and is often presented with lots of mathematical formality.

The math is not very important for our purposes, but you should check it out if you get serious about solving regression problems.



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But again, if you get serious about regression, you should learn how this works!

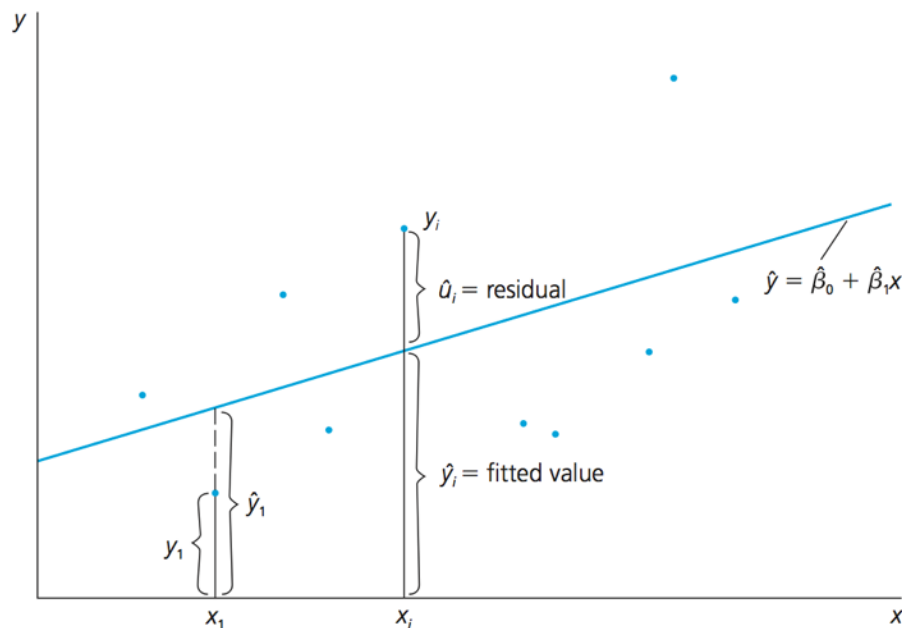
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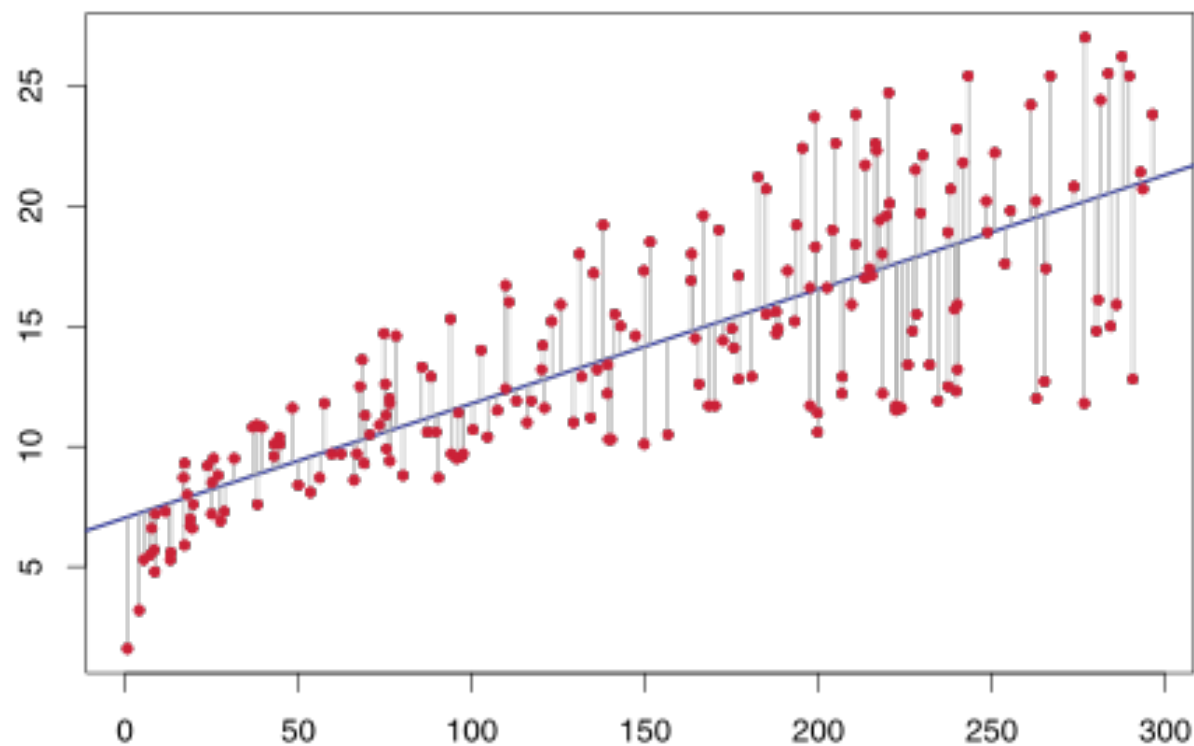
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i.$$

$$\hat{u}_i = y_i - \hat{y}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i.$$

$$\sum_{i=1}^n \hat{u}_i^2 = \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2,$$



LINEAR REGRESSION



$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x,$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2},$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x},$$

II: POLYNOMIAL REGRESSION

*Consider the following **polynomial regression model**:*

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“Although polynomial regression fits a nonlinear model to the data, as a statistical estimation problem it is linear, in the sense that the regression function $E(y|x)$ is linear in the unknown parameters that are estimated from the data. For this reason, polynomial regression is considered to be a special case of multiple linear regression.” -- Wikipedia

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Q: Does anyone know what it is?

A: This model violates one of the assumptions of linear regression!



This model displays multicollinearity, which means the predictor variables are highly correlated with each other.

$$y = \alpha + \beta_1 x + \beta_2 x^2 + \dots + \beta_n x^n + \varepsilon$$

```
> x <- seq(1, 10, 0.1)
> cor(x^9, x^10)
[1] 0.9987608
```

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$$y = \alpha + \beta_1 x + \beta_2 x^2 + \dots + \beta_n x^n + \varepsilon$$

Multicollinearity causes the linear regression model to break down, because it can't tell the predictor variables apart.

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OPTIONAL NOTE

These polynomial functions form an *orthogonal basis* of the function space.

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Q: Can a regression model be too complex?

III: REGULARIZATION

*Recall our earlier discussion of **overfitting**.*

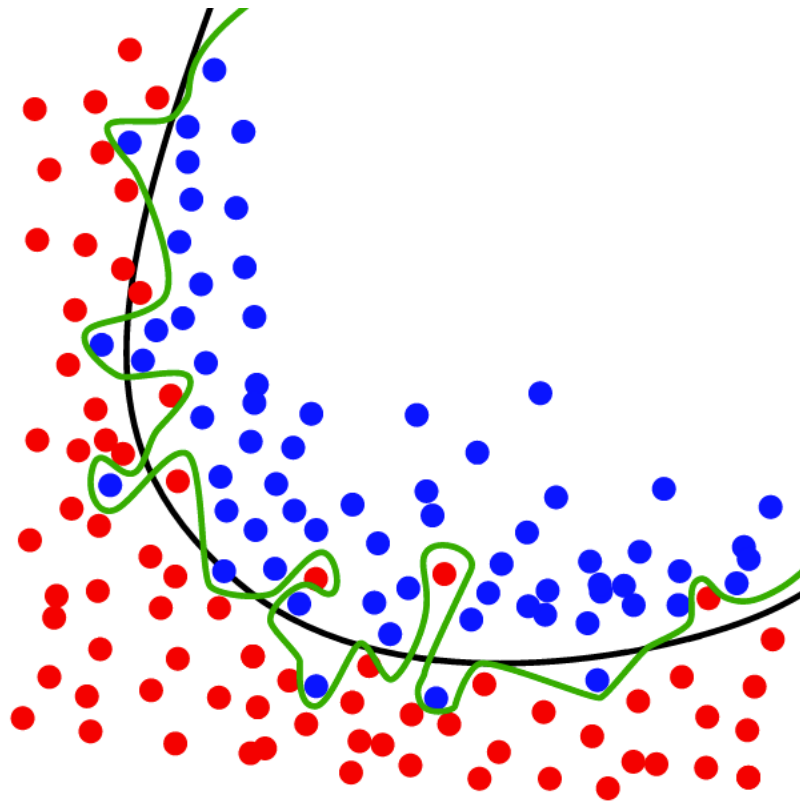
*Recall our earlier discussion of **overfitting**.*

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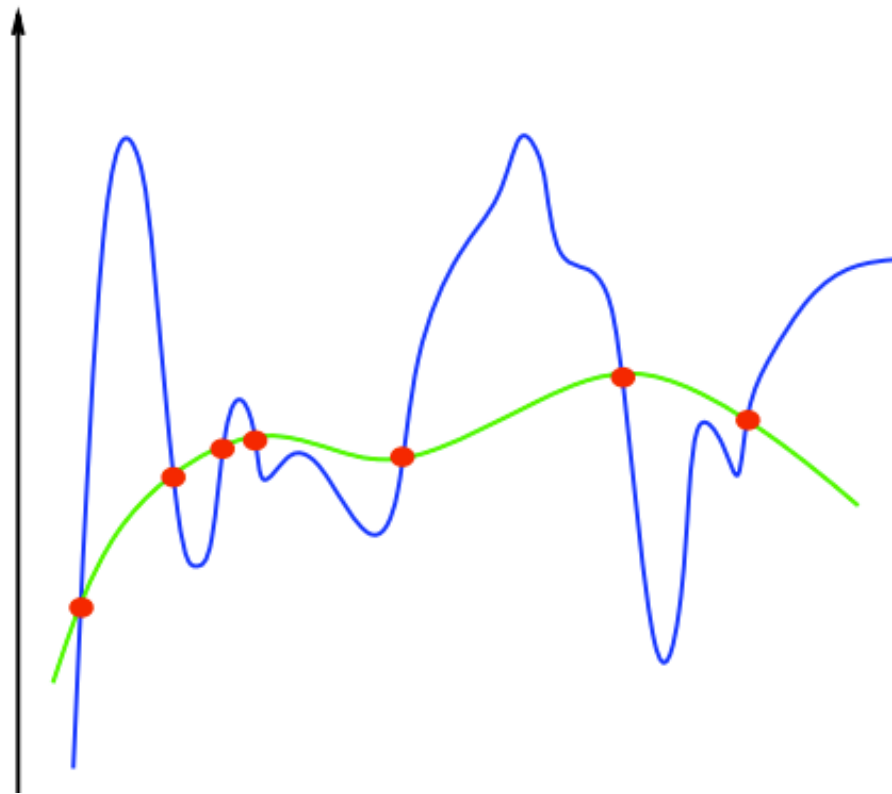
*In other words, an overfit model matches the **noise** in the dataset instead of the **signal**.*



The same thing can happen in regression.

It's possible to design a regression model that matches the noise in the data instead of the signal.

This happens when our model becomes too complex for the data to support.



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A: One method is to define complexity as a function of the size of the coefficients.

*Ex 1: $\sum |\beta_i|$ this is called the **L1-norm***

*Ex 2: $\sum \beta_i^2$ this is called the **L2-norm***

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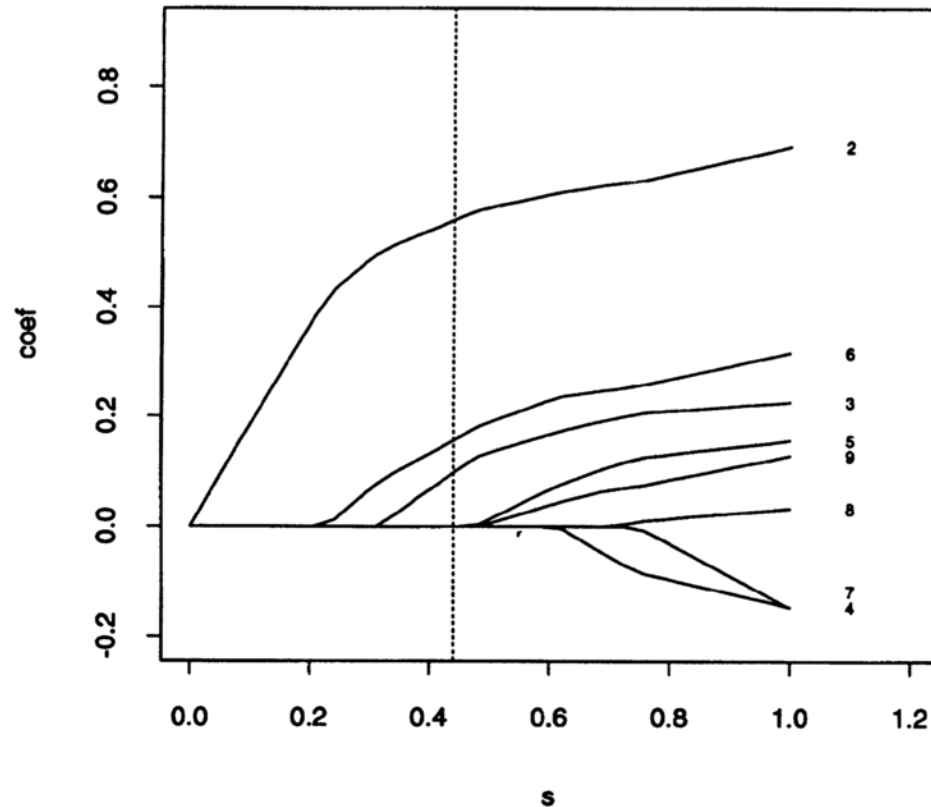
Regularization *refers to the method of preventing overfitting by explicitly controlling model complexity.*

These regularization problems can also be expressed as:

L1 regularization (Lasso): $\min(\|y - x\beta\|^2 + \lambda\|x\|)$

L2 regularization (Ridge): $\min(\|y - x\beta\|^2 + \lambda\|x\|^2)$

This (Lagrangian) formulation reflects the fact that there is a cost associated with regularization.



As the regularization parameter (s in this chart, λ on the previous slide) goes to zero, so do the coefficients of the features

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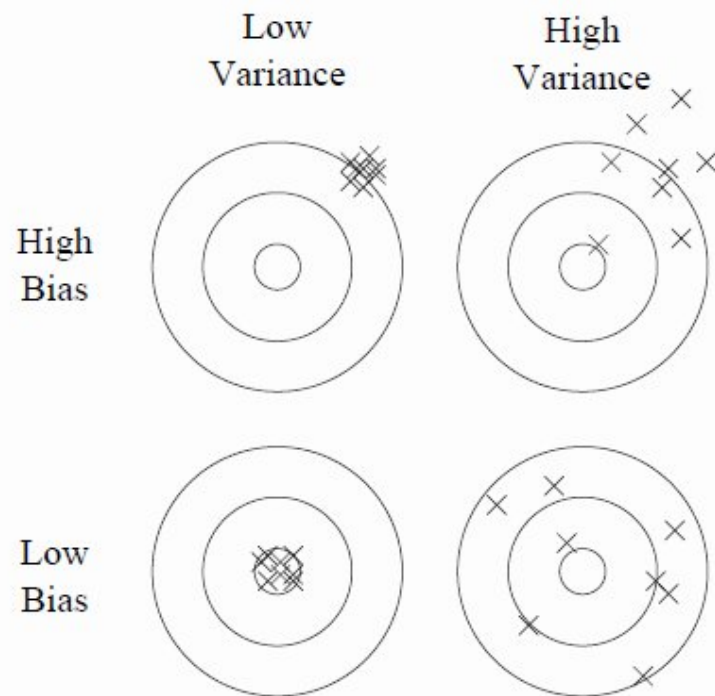


Figure 1: Bias and variance in dart-throwing.

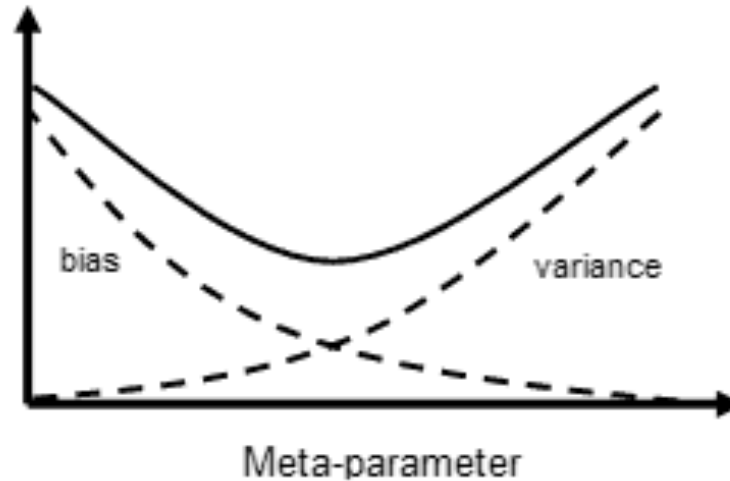
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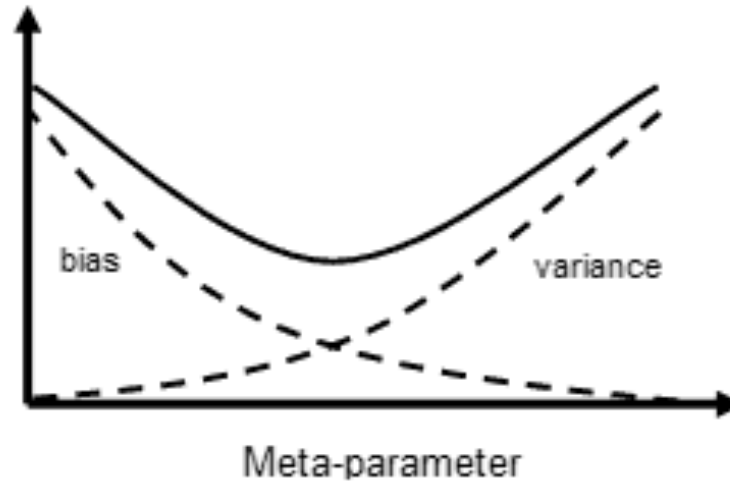
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It turns out (after some math) that the generalization error in our model can be decomposed into a bias component and variance component.

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**NOTE**

The “meta-parameter” here is the λ we saw above.

A more typical term is “hyperparameter”.

*This tradeoff is regulated by a **hyperparameter** λ , which we've already seen:*

L1 regularization: $y = \sum \beta_i x_i + \varepsilon \quad \text{st.} \quad \sum |\beta_i| < \lambda$

L2 regularization: $y = \sum \beta_i x_i + \varepsilon \quad \text{st.} \quad \sum \beta_i^2 < \lambda$

So regularization represents a method to trade away some variance for a little bias in our model, thus achieving a better overall fit.

- *Linear regression*
- *Multiple regression*
- *Polynomial regression*
- *The concept of minimizing some error or “cost” function*
- *Regularization*

INTRO TO DATA SCIENCE

LAB: REGRESSION & REGULARIZATION