Understanding, Evaluating, and Generating Prediction Intervals

(In regression contexts with a frequentist orientation)

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Data Science @NetApp

posit conf (2024)

github.com/brshallo/posit-2024

bryanshalloway.com

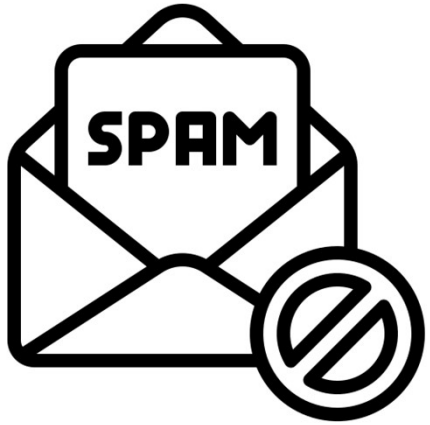
Rooftop solar's dark side

JULY 12, 2024 · 6:28 PM ET

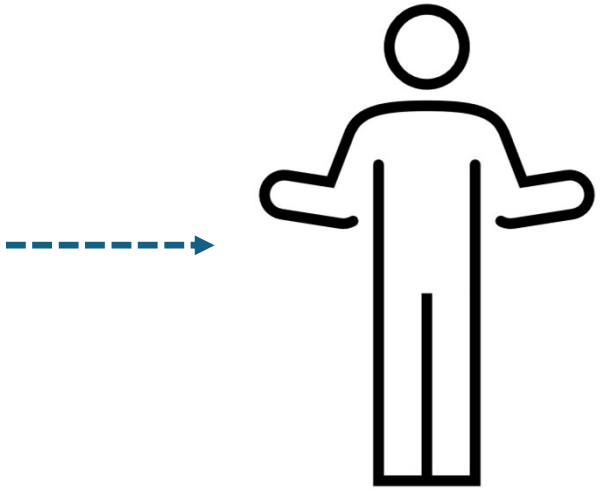
"They had used about half as much electricity from their power company as the previous year..."

"But {the solar company} had promised these new panels would replace all of their power."

$$\hat{f}(x_i)$$

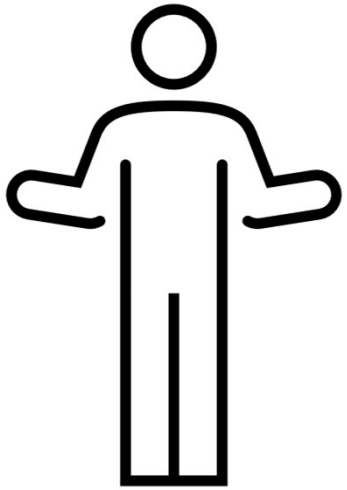


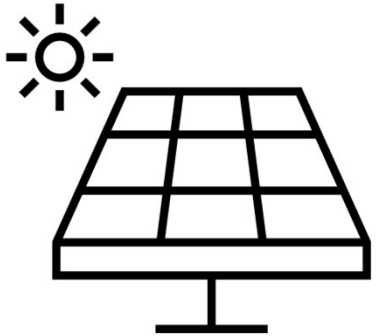
$\hat{f}(x_i)$



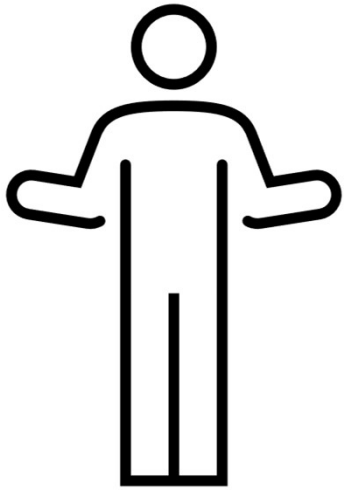
...

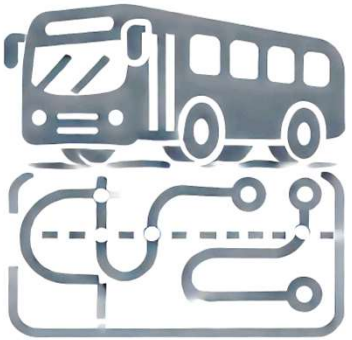
$$\hat{f}(x_i)$$



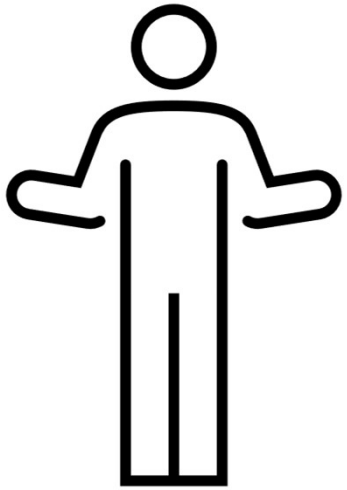


$\hat{f}(x_i)$

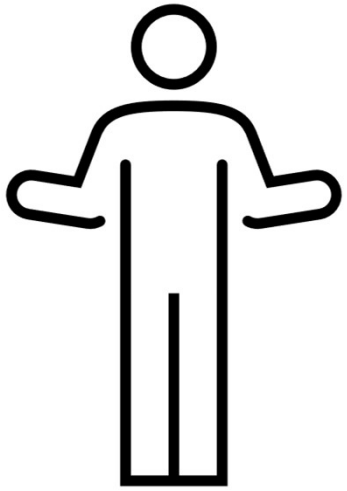




$$\hat{f}(x_i)$$



$\hat{f}(x_i)$ ...



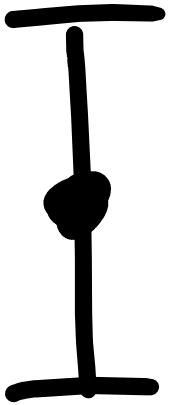
$\hat{f}(x_i)$ ...

- Applicability → Is the model appropriate to use for this observation?
- Explainability → What attributes are driving the predicted value?
- Uncertainty → What's a reasonable range for this outcome?
- ...

Point Estimate

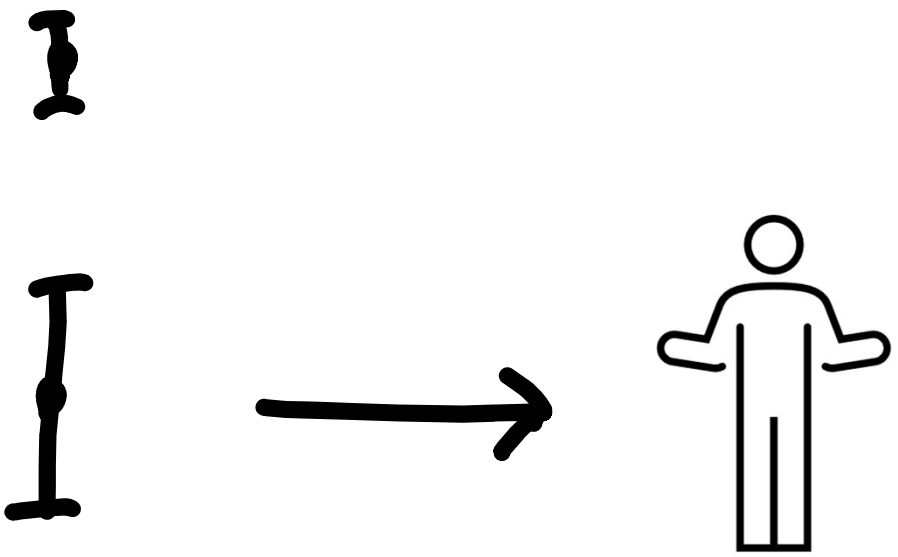
"This car will sell for $12k"

Prediction Interval

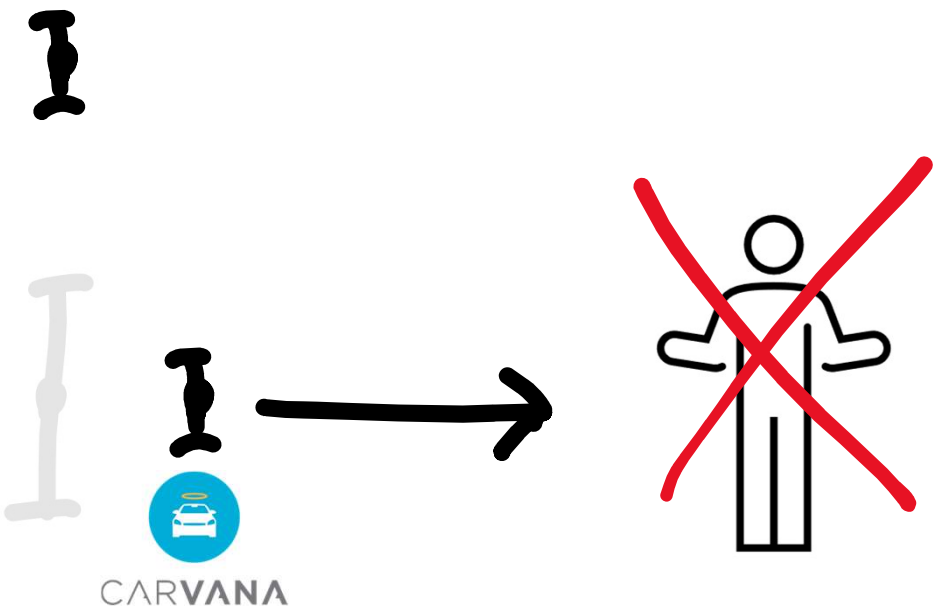


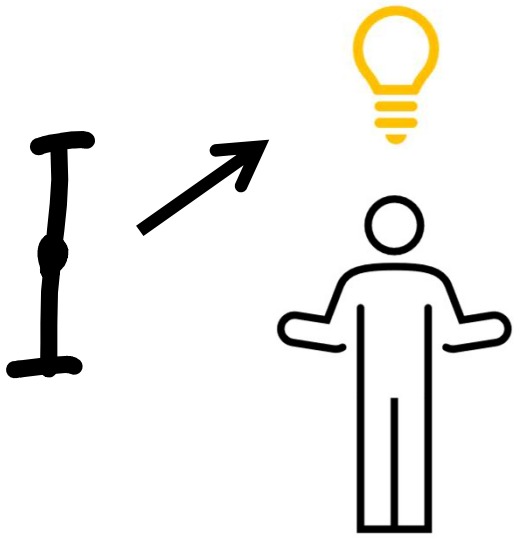
"I'm 80% sure this car will sell for between $10k and $14k"

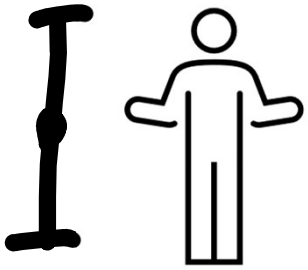
$\hat{f} \longrightarrow \$\$$

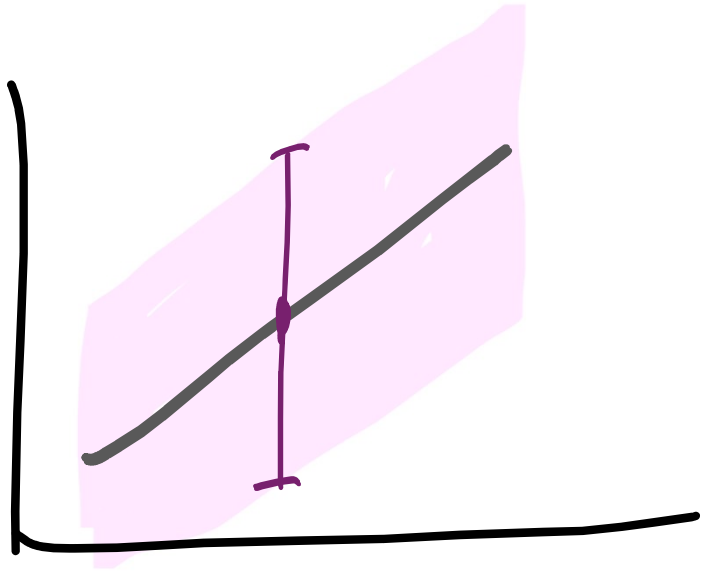


$\hat{f} \longrightarrow \$\$$

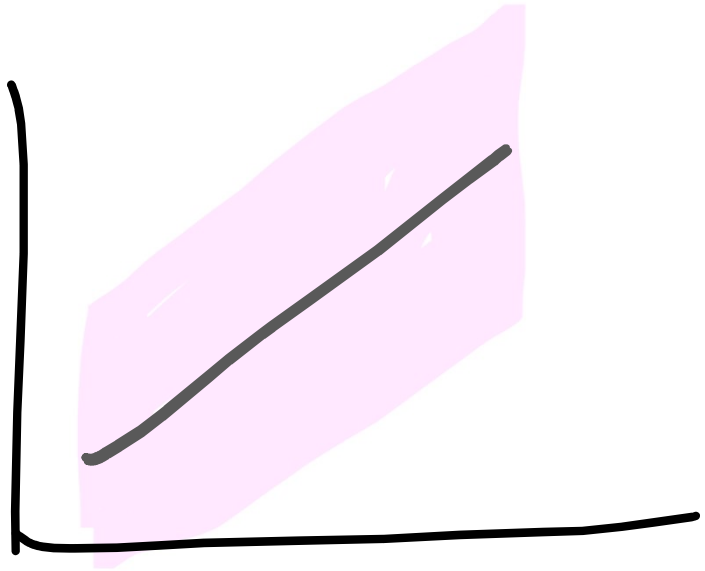




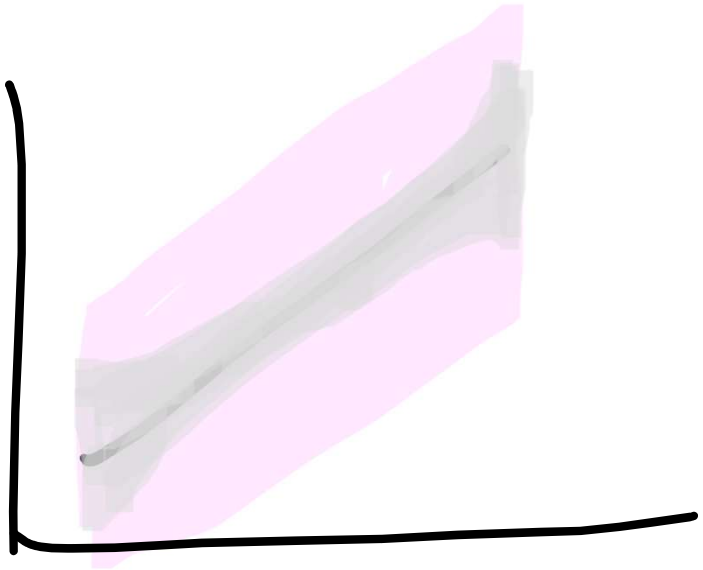




Confidence Intervals vs Prediction Intervals

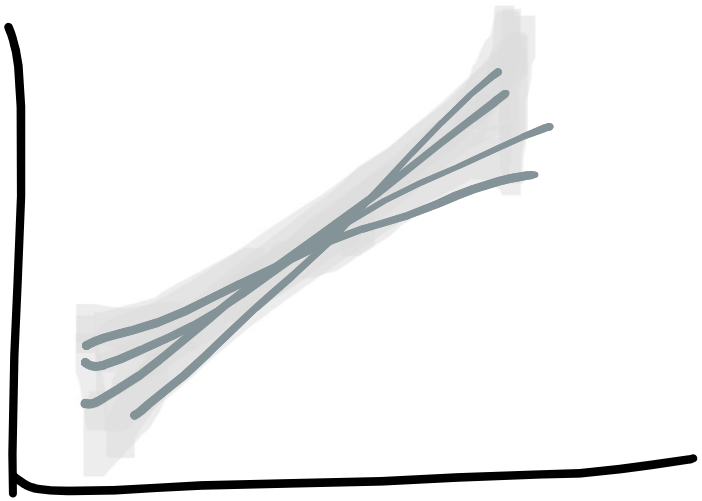


Confidence Intervals vs Prediction Intervals

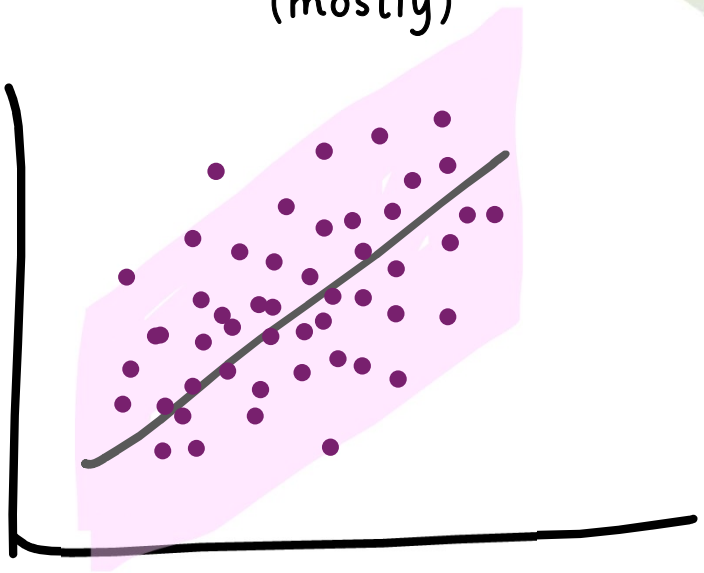


Confidence Intervals vs Prediction Intervals

Uncertainty in Fitting Model
(mostly)



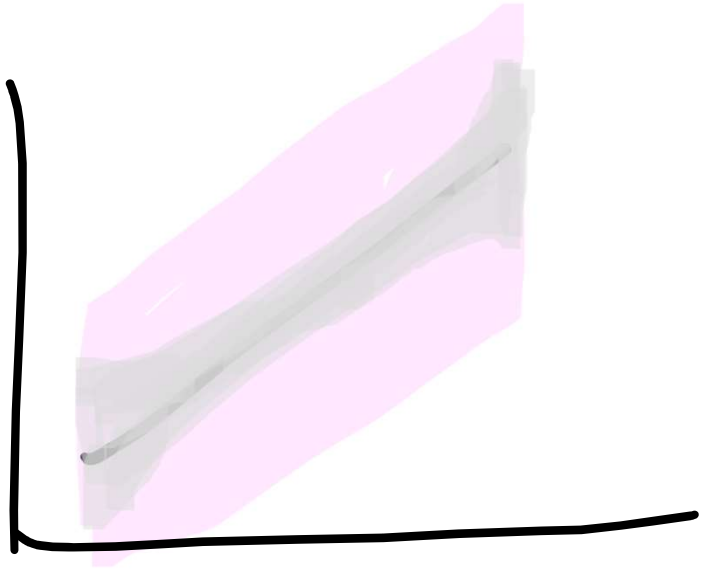
Uncertainty in Sample
(mostly)



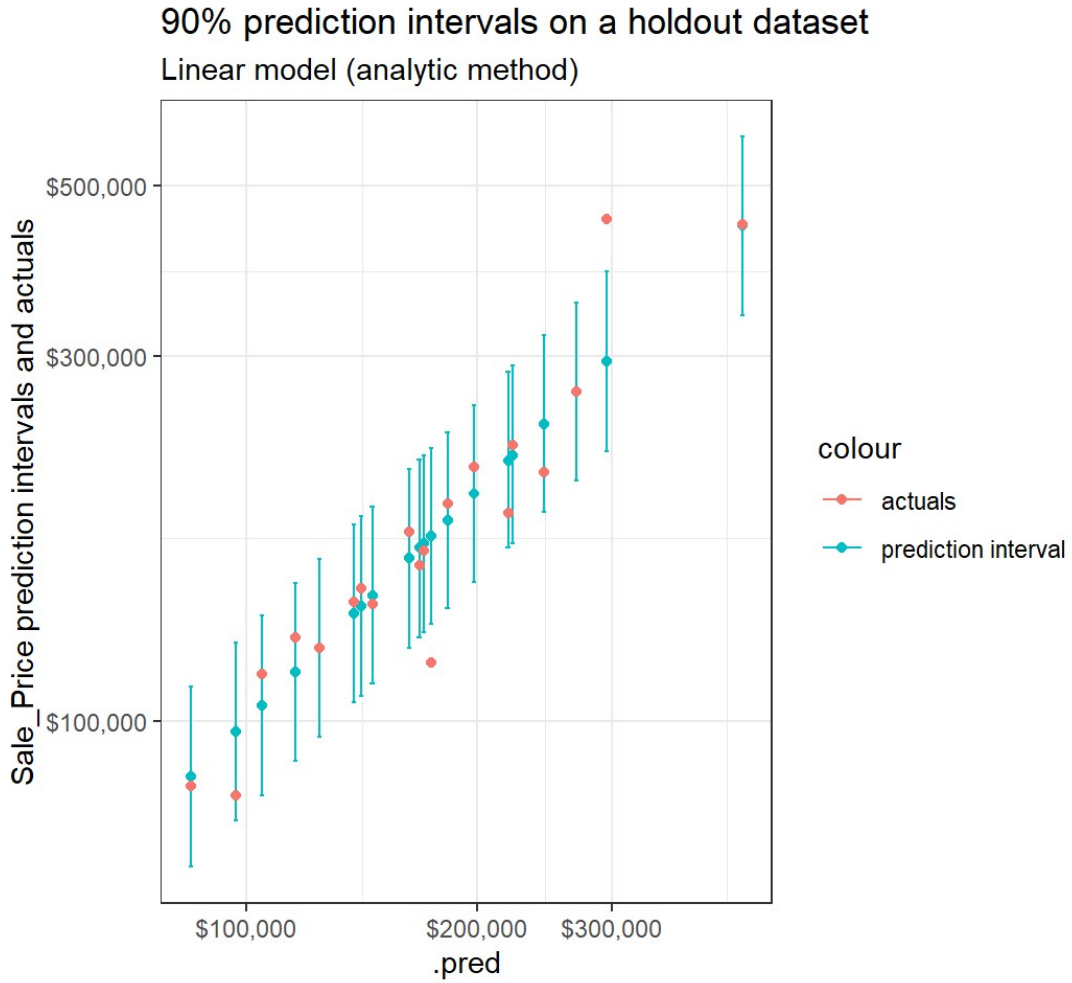
Confidence Intervals vs Prediction Intervals

90% sure the average weight among all 3 mo olds is 12 - 12.5 lbs

90% sure the weight of an individual random 3 mo old will be 10 - 14 lbs

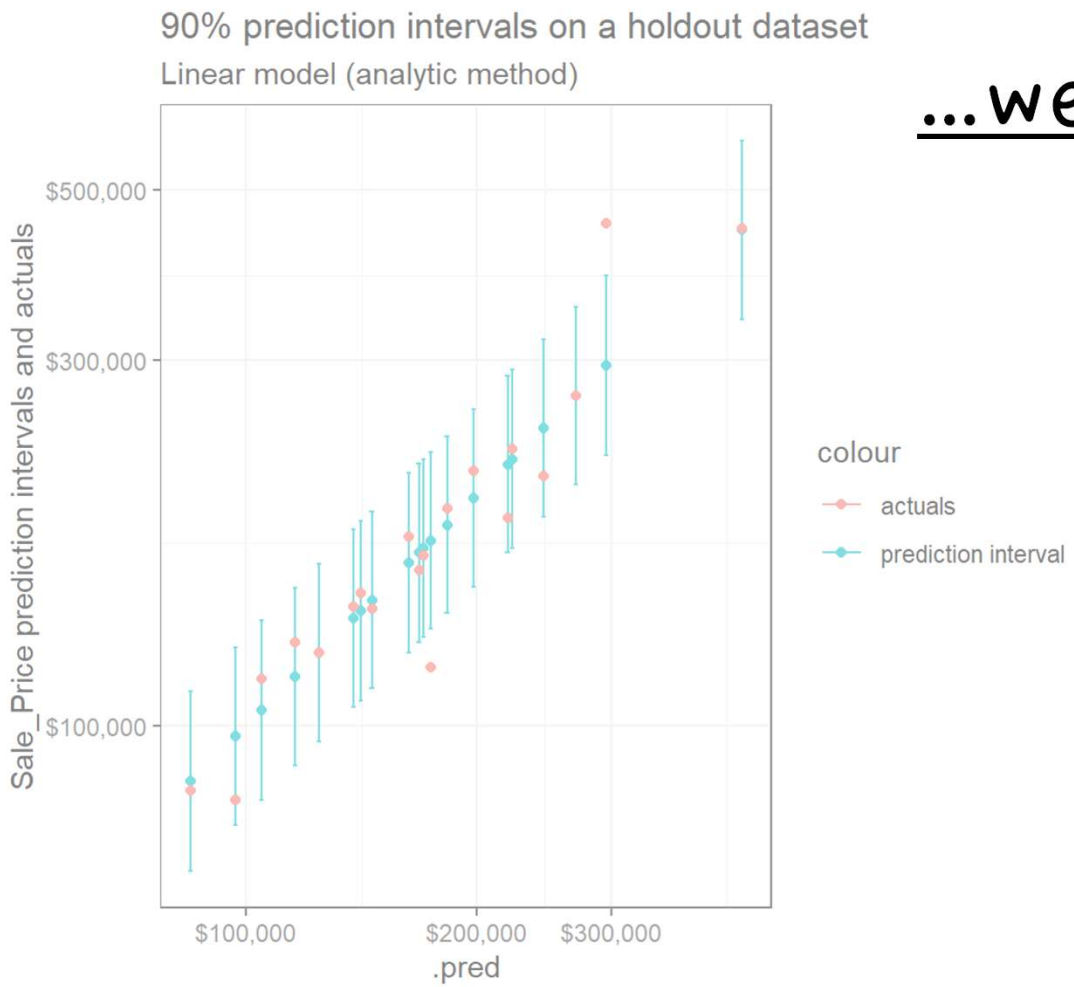


```
predict(lm_fit, data_test,
        type = "pred_int",
        level = 0.90)
#> # A tibble: 14 × 2
#>    .pred_lower .pred_upper
#>          <dbl>       <dbl>
#>  1        17.6        24.5
#>  2        18.5        25.4
#>  3        18.6        25.5
#>  4        18.8        25.7
#>  5        18.1        25.1
#>  6         4.19       11.2
#>  7         2.72        9.67
#>  8        17.0        23.9
#>  9        18.4        25.3
#> 10        18.4        25.3
#> 11        18.4        25.3
#> 12        17.7        24.6
#> 13         5.27       12.2
#> 14         4.26       11.2
```



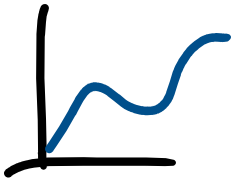
- coverage
- interval width
- ...

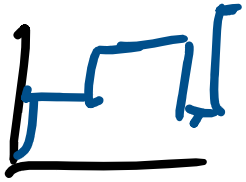
...weaknesses


90% prediction intervals on a holdout dataset
Linear model (analytic method)
Sale_Price prediction intervals and actuals
$500,000
$300,000
$100,000
$100,000
$200,000
$300,000
.pred
colour
actuals
prediction interval

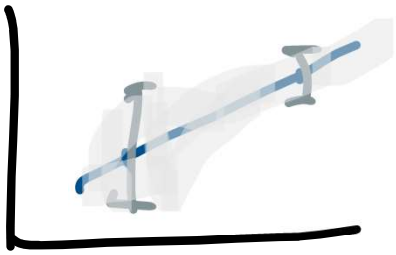
...weaknesses

- No guarantee of coverage





- Other model types



- Assumptions

...

desired...

- Coverage guaranteed
- Model Agnostic
- Assumption free (and flexible)

...weaknesses

- No guarantee of coverage
- Other model types
- Assumptions
- ...

Conformal Prediction

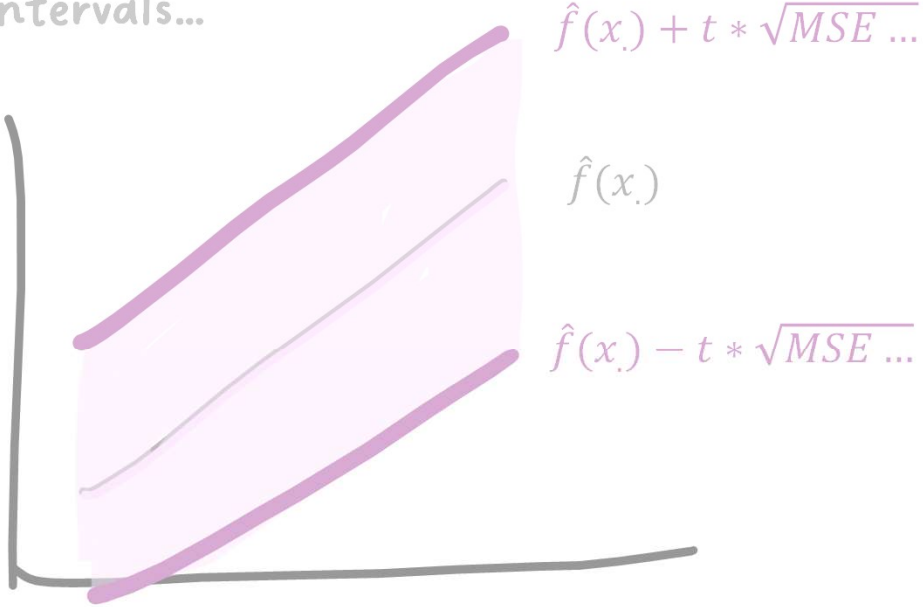
(Mostly) assumption free uncertainty quantification

Conformalized quantile regression is...
"the best way to do conformal prediction for regression."
-Stephen Bates
coauthor of A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification

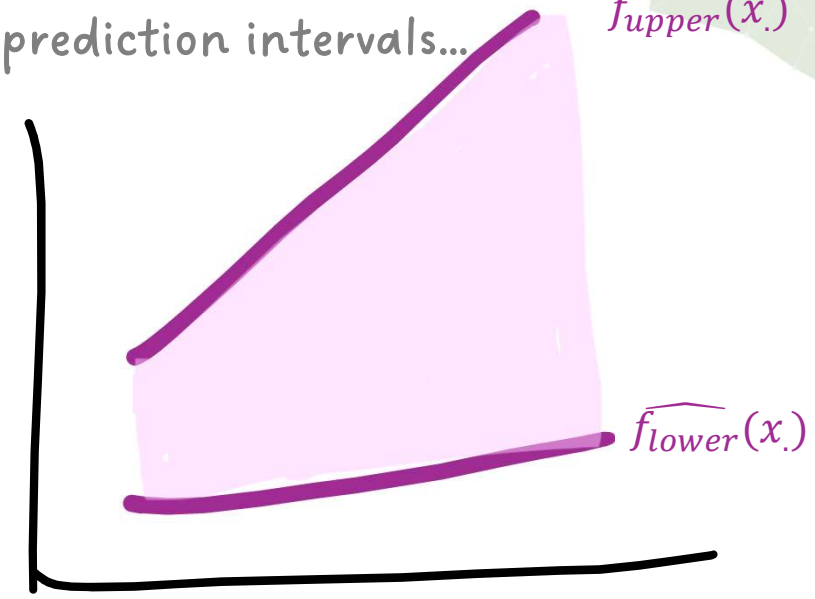
1. *Fit models for upper and lower bounds using quantile regression*
2. *Adjust bounds using calibration data*

1. Don't fit expected values, but quantiles

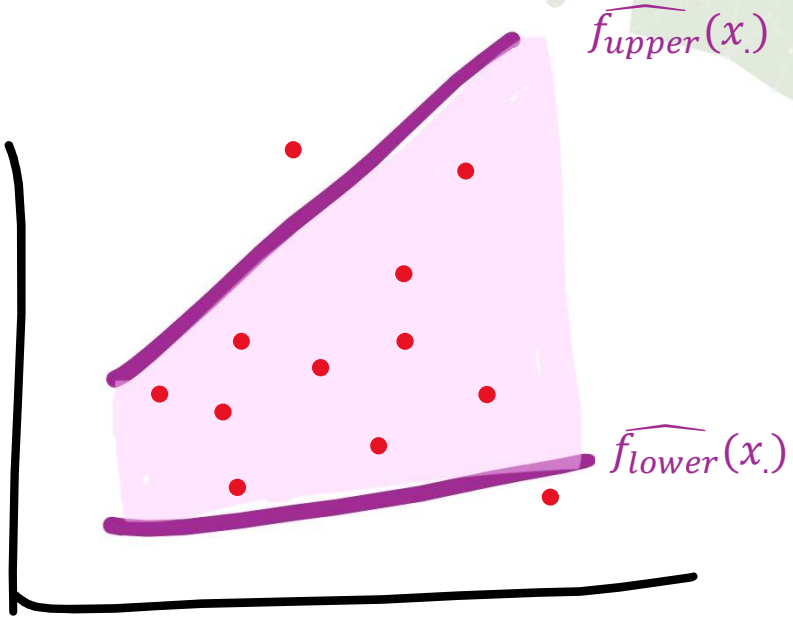
Classical prediction intervals...



Quantile based prediction intervals...



2. Calibrate, adjust bounds



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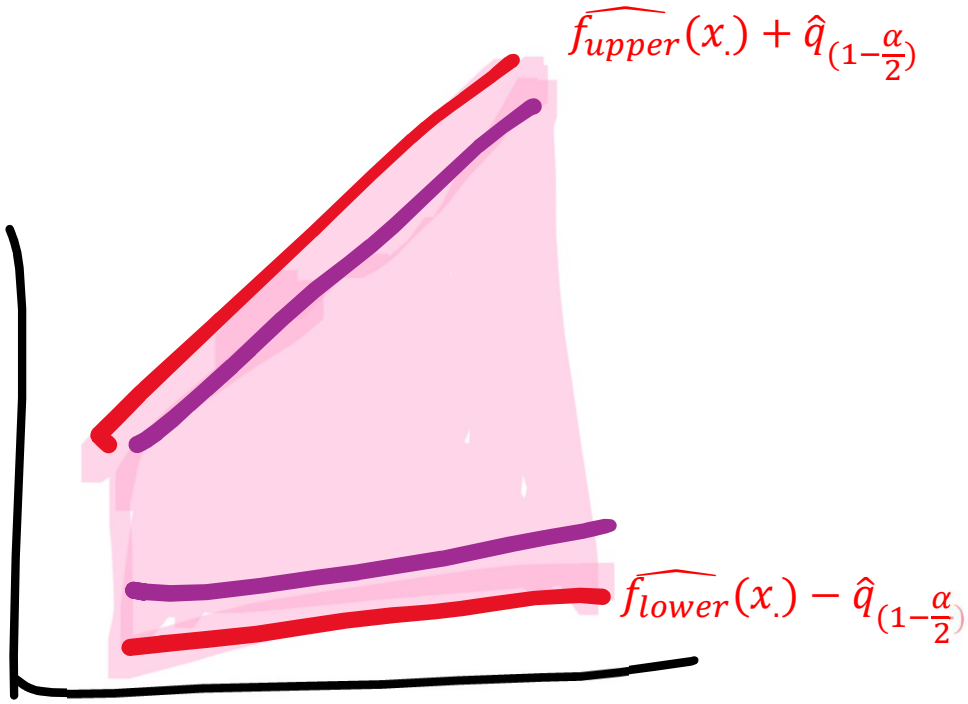
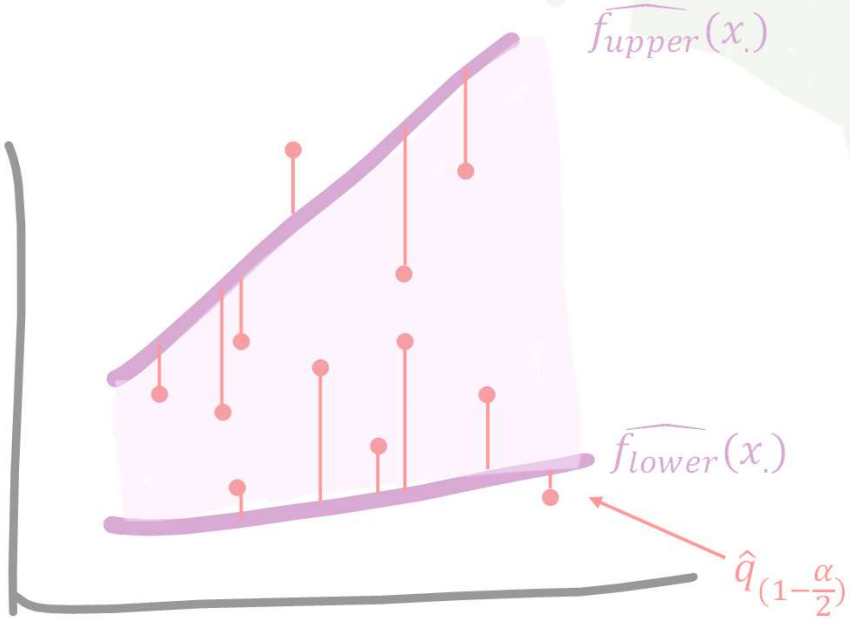




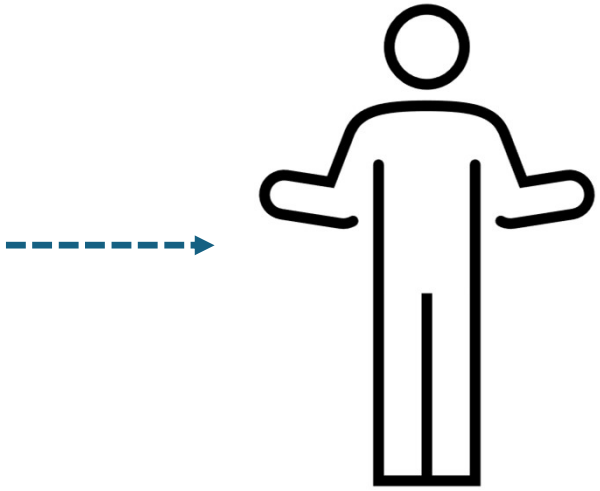
Conformalized Quantile Regression Resources

- `probably::int_conformal_quantile()`
  Conformal Inference with Tidymodels - posit::conf(2023); *Kuhn* (https://youtu.be/vJ4BYJSg734?si=cjpXabfmAad1FuBK)
- MAPIE: Model Agnostic Prediction Interval Estimator (python)
  https://mapie.readthedocs.io/en/latest/
- A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification; *Angelopoulos, Bates* (https://people.eecs.berkeley.edu/~angelopoulos/blog/posts/gentle-intro/)
- Introduction To Conformal Prediction with Python; *Molnar*
- Practical Guide to Applied Conformal Prediction...; *Manokhin*

Also:

- Understanding Prediction Intervals; *Shalloway* (https://www.bryanshalloway.com/2021/03/18/intuition-on-uncertainty-of-predictions-introduction-to-prediction-intervals/)

$\hat{f}(x_i)$



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