

Quantitative Predictive Check (QPC) scoring for VPC

Introduction

A Visual Predictive Check (VPC) is typically assessed visually by checking:

- calibration (are observations inside simulated prediction intervals?)
- bias and trend (does the model systematically miss in certain x regions?)
- sharpness (are prediction intervals unnecessarily wide?)

The **Quantitative Predictive Check (QPC)** score in `tidyvpc` is a *numeric* summary of these features, computed from an existing `tidyvpcobj` after `vpcstats()`.

QPC produces a table `qpc.stats` and a composite scalar `qpc_score` (**lower is better**) that can be used for automated model comparison and optimization.

What QPC measures (methodology overview)

QPC is computed from `o$stats` (the `data.table` produced by `vpcstats()`), which contains (for continuous VPCs) curve points across quantiles:

- `qname`: quantile curve (e.g. `q0.05`, `q0.5`, `q0.95`)
- `y`: observed curve value at `x`
- `md`: simulated median curve at `x`
- `lo`, `hi`: simulated confidence interval bounds at `x` for that quantile curve

At each curve point, QPC derives:

- **Coverage**: whether $y \in [lo, hi]$
- **Deviation**: $|y - md|$ relative to PI half-width
- **Drift**: Spearman correlation of residuals $(y - md)$ versus `x` (monotonic bias)
- **Sharpness**: interval width (penalizes “variance inflation”)
- **Proper interval score (Winkler)**: rewards narrow intervals but penalizes misses

These are aggregated across curves and combined into `qpc_score` with user-controlled weights.

Penalties (what is printed)

`qpcstats()` prints a scalar `qpc_score` plus a component breakdown. Each component is designed to be **0 = best** and larger values = worse.

At a high level:

- **Coverage penalties** measure calibration (are observed curves inside simulated uncertainty bands?).

- **MAE and drift penalties** measure agreement and bias structure (how far and whether the residuals trend with x).
- **Sharpness and interval penalties** discourage “variance inflation” (overly wide bands that can artificially increase coverage).

More concretely (continuous VPC):

- **Median coverage penalty** (`coverage_penalty_med`): computed from the median quantile curve (the curve closest to $q = 0.5$):

$$1 - \text{mean}(\mathbf{1}[y \in [lo, hi]])$$

Lower is better; 0 means the observed median curve is always inside the simulated band.

- **Tail coverage penalty** (`coverage_penalty_tails`): computed from the lowest and highest quantile curves available (typically $q = 0.05$ and $q = 0.95$), averaged:

$$\frac{(1 - \text{coverage}_{low}) + (1 - \text{coverage}_{high})}{2}$$

- **MAE penalty** (`mae_penalty_all`): based on deviation scaled by PI half-width:

$$dev_mid = \frac{|y - md|}{(hi - lo)/2}$$

then bounded to $[0, 1]$ and averaged across curves. This highlights “large misses relative to the model’s own uncertainty”.

- **Drift penalty** (`rho_penalty_all`): absolute Spearman correlation of residuals $(y - md)$ vs x (averaged across curves), bounded to $[0, 1]$. Values near 0 indicate no monotonic bias trend across x; larger values indicate systematic drift.
- **Sharpness penalty** (`sharpness_penalty`): penalizes wide bands using relative width:

$$width_rel = \frac{(hi - lo)}{|md|}$$

By default (single-VPC scoring), this is mapped to $[0, 1]$ with a bounded transform:

$$1 - e^{-\max(width_rel, 0)}$$

Optionally, you can anchor this with `sharp_ref` for cross-model comparability.

- **Interval penalty** (`interval_penalty`): based on the Winkler interval score for nominal PI level $(1 - \alpha)$:

$$IS = (hi - lo) + \frac{1}{2} \alpha (lo - y) \mathbf{1}[y < lo] + \frac{1}{2} \alpha (y - hi) \mathbf{1}[y > hi]$$

This rewards narrow intervals but strongly penalizes misses. By default we apply a bounded transform to a normalized score; optionally you can anchor with `interval_ref`.

Finally:

$$qpc_score = \sum_i w_i \cdot penalty_i$$

where `w` is the named weight vector (`med_cov`, `tail_cov`, `mae`, `drift`, `sharp`, `interval`).

Data

We'll use the built-in `tidyvpc::obs_data` and `tidyvpc::sim_data` and follow the standard preprocessing used throughout our vignettes.

```
obs_data <- as.data.table(tidyvpc::obs_data)
sim_data <- as.data.table(tidyvpc::sim_data)

obs_data <- obs_data[MDV == 0]
sim_data <- sim_data[MDV == 0]
```

Add the population prediction PRED (from replicate 1) into the observed data for pcVPC examples:

```
obs_data$PRED <- sim_data[REP == 1, PRED]
```

Example 1: Basic QPC scoring

Below is a standard continuous VPC using binless VPC stats. The QPC computation is a post-processing step after `vpcstats()`.

```
vpc <- observed(obs_data, x = TIME, y = DV) %>%
  simulated(sim_data, y = DV) %>%
  binless() %>%
  vpcstats()

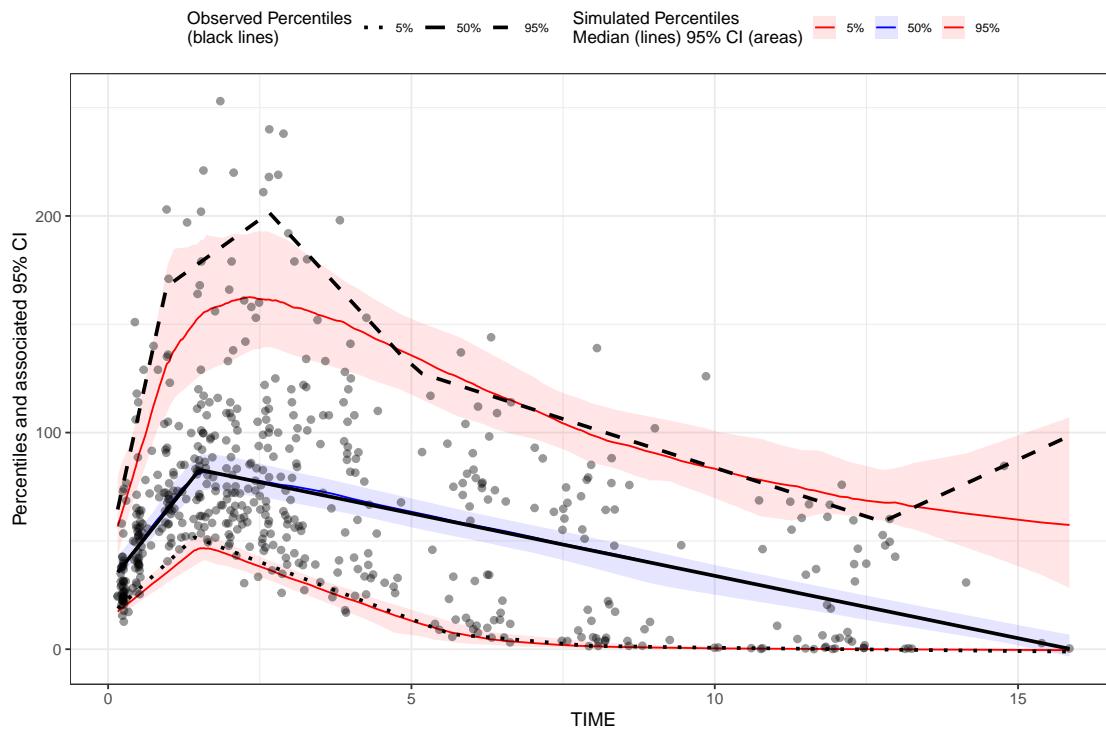
vpc <- qpcstats(vpc)

print(vpc)
#> VPC with 100 replicates
#> Stratified by:
#> QPC: qpc_score = 0.159 (lower is better)
#> Breakdown (0 = best):
#>   median coverage penalty  0.000
#>   tail coverage penalty   0.092
#>   MAE penalty             0.221
#>   drift penalty           0.409
#>   sharpness penalty       0.272
#>   interval penalty        0.391
#>
#>          x  qname      y      md      lo      hi
#>          <num> <fctr>  <num>  <num>  <num>  <num>
#>  1: 0.2157624 q0.05 20.27050 18.70099 15.46726 22.76529
#>  2: 0.4694366 q0.05 26.85172 24.20164 20.90806 28.69981
#>  3: 0.8271844 q0.05 36.13299 32.25889 27.80422 37.28306
#>  4: 1.7724895 q0.05 47.97810 45.68455 39.37618 51.15900
#>  5: 1.7142415 q0.05 48.59415 46.13059 39.92622 51.83491
#>  ---
#> 1646: 3.1146520 q0.95 187.64868 157.66057 135.21747 185.70608
#> 1647: 3.9526689 q0.95 162.26683 149.76519 128.25975 168.88196
#> 1648: 6.0247591 q0.95 119.55945 122.36560 105.29532 140.59213
#> 1649: 7.7967326 q0.95 103.60993 101.08928 88.41343 115.52899
#> 1650: 12.2981243 q0.95 63.09294 69.37852 61.51805 85.95328
```

The composite score is available in `qpc.stats$qpc_score` (for stratified VPCs you will also see an `qpc_scope == "overall"` row).

Plot the VPC:

```
plot(vpc)
```



Example 2: QPC with prediction correction and stratification

QPC relies on `vpc$stats`, so it naturally works with prediction correction and stratification (for continuous VPCs).

```
vpc_pc_strat <- observed(obs_data, x = TIME, y = DV) %>%
  simulated(sim_data, y = DV) %>%
  stratify(STUDY ~ GENDER) %>%
  predcorrect(pred = PRED) %>%
  binless() %>%
  vpcstats()

vpc_pc_strat <- qpcstats(vpc_pc_strat)
print(vpc_pc_strat)
#> Prediction corrected VPC with 100 replicates
#> Stratified by: STUDY, GENDER
#> QPC: qpc_score = 0.148 (lower is better)
#> Breakdown (0 = best):
#>   median coverage penalty  0.009
#>   tail coverage penalty    0.037
#>   MAE penalty              0.201
```

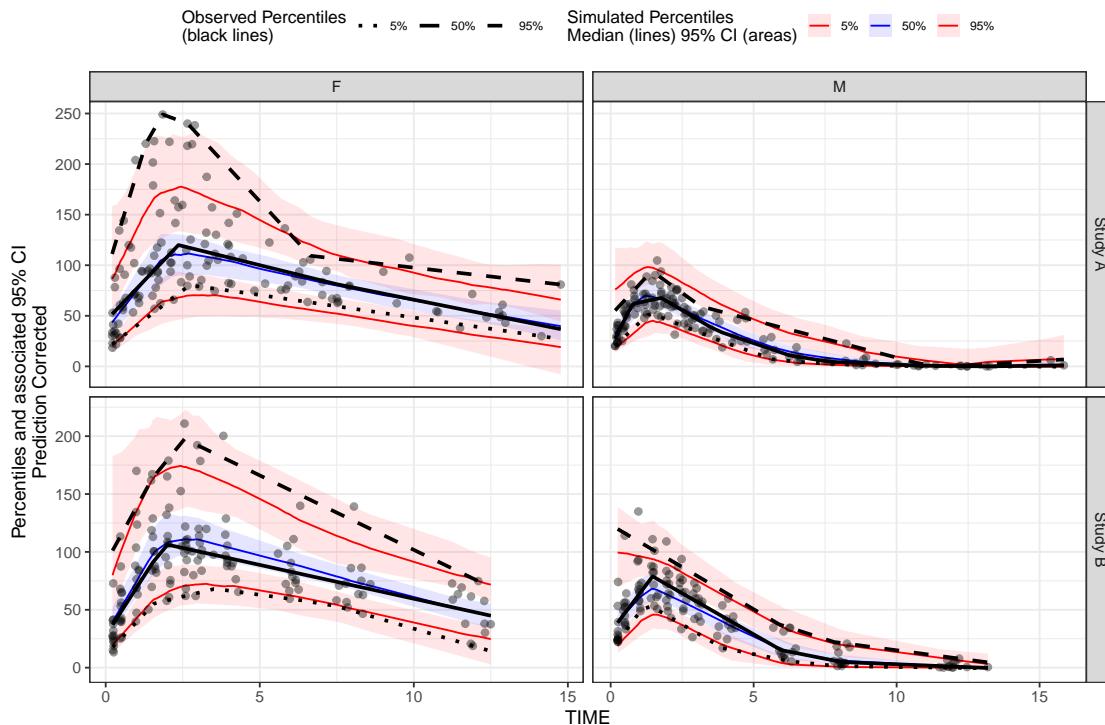
```

#>   drift penalty          0.078
#>   sharpness penalty      0.453
#>   interval penalty       0.542
#>
#> # QPC qpc_score by stratum:
#>   STUDY GENDER qpc_score qpc_scope
#>   <char> <char> <num> <char>
#> 1: Study A      F 0.2185022 stratum
#> 2: Study B      F 0.1143301 stratum
#> 3: Study A      M 0.1760193 stratum
#> 4: Study B      M 0.1995141 stratum
#> 5: __ALL__ __ALL__ 0.1481005 overall
#>
#>           x  qname  STUDY GENDER      y      md      lo      hi
#>           <num> <fctr> <char> <char>  <num>  <num>  <num>  <num>
#> 1: 0.2414537 q0.05 Study A      F 22.628106 21.603303 14.635225 29.01338
#> 2: 0.6153070 q0.05 Study A      F 31.298883 31.217977 22.157131 43.88344
#> 3: 0.7493947 q0.05 Study A      F 34.408780 34.786598 25.021506 49.07117
#> 4: 1.6711424 q0.05 Study A      F 55.786869 59.999193 39.790871 82.52384
#> 5: 2.2418821 q0.05 Study A      F 69.024031 66.798270 45.272725 93.57229
#> ---
#> 1646: 2.9649190 q0.95 Study B      M 80.150799 75.984410 61.464186 97.94624
#> 1647: 4.2881855 q0.95 Study B      M 60.858937 58.079728 43.476314 75.06576
#> 1648: 6.0457983 q0.95 Study B      M 36.202388 34.662559 21.504472 51.58254
#> 1649: 7.9075620 q0.95 Study B      M 21.905414 20.454721 11.120393 34.17353
#> 1650: 12.0612380 q0.95 Study B      M 8.275706 6.636687 2.630895 14.68703

```

Plot the stratified pcVPC:

```
plot(vpc_pc_strat)
```



Interpreting differences between vpc and vpc_pc_strat

In the vignette examples you printed:

- The **prediction-corrected + stratified** VPC (`vpc_pc_strat`) shows a **lower drift penalty** (residuals trend less with x), because prediction correction and stratification often remove structured bias that would otherwise appear as monotonic drift.
- At the same time, `vpc_pc_strat` can show **higher sharpness/interval penalties** if the simulated uncertainty bands are wider within strata (or if prediction correction changes the scale/structure of residuals), because QPC explicitly penalizes overly wide intervals even when they improve coverage.
- The **per-stratum qpc_score table** helps localize which subpopulations drive the overall score: strata with worse calibration (coverage penalties) or wider uncertainty (sharpness/interval penalties) will typically have higher `qpc_score`.

Example 3: QPC scoring with traditional binning()

QPC works with traditional binned VPCs as well (it scores directly from `vpc$stats`). The only difference is that `vpcstats()` will compute summaries at `xbin` instead of `x`.

```
vpc_binned <- observed(obs_data, x = TIME, y = DV) %>%
  simulated(sim_data, y = DV) %>%
  binning(bin = NTIME) %>%
  vpcstats()

vpc_binned <- qpcstats(vpc_binned)

print(vpc_binned)
#> VPC with 100 replicates
#> Stratified by:
#> QPC: qpc_score = 0.149 (lower is better)
#> Breakdown (0 = best):
#>   median coverage penalty  0.000
#>   tail coverage penalty   0.091
#>   MAE penalty             0.199
#>   drift penalty            0.276
#>   sharpness penalty        0.311
#>   interval penalty         0.428
#>
#> Key: <xbin>
#>       bin      xbin  qname      y          lo          md          hi
#>       <fctr>    <num> <fctr>    <num>      <num>      <num>      <num>
#> 1:  0.25  0.2490835 q0.05 17.4250 13.20370500 16.63365000 20.0638487
#> 2:  0.25  0.2490835 q0.5 28.1000 26.33373750 30.44625000 36.4071750
#> 3:  0.25  0.2490835 q0.95 70.9100 47.45008250 55.05687500 71.2563250
#> 4:  0.5   0.5009004 q0.05 28.9200 24.25121000 29.00000000 35.0677837
#> 5:  0.5   0.5009004 q0.5 51.8000 46.10241250 51.90550000 60.0179125
#> ---
#> 29:     8  8.0691507 q0.5 35.0000 24.03068750 33.87400000 42.8817250
#> 30:     8  8.0691507 q0.95 95.7900 83.68695000 96.48842500 110.8845750
#> 31:    12 12.0253628 q0.05  0.1291  0.02170331  0.08714695  0.2521808
#> 32:    12 12.0253628 q0.5 13.3750  7.52458375 15.91905000 24.0568625
#> 33:    12 12.0253628 q0.95 67.5600 59.34408250 68.91725000 82.5615012
```

Example 4: Noisy simulations → wider confidence intervals → worse QPC

One failure mode of purely visual scoring is that *very wide* simulated confidence intervals can appear to “cover everything”. QPC penalizes this via **sharpness** and **interval score** components.

Here we artificially add noise to the simulated DV values to create wider confidence intervals, then compare `qpc.stats`.

```
sim_data_noisy <- copy(sim_data)

# Increase variability of simulated DV values; this should widen lo/hi bands.
sim_data_noisy[, DV := DV + rnorm(.N, mean = 0, sd = 25)]

vpc_base <- observed(obs_data, x = TIME, y = DV) %>%
  simulated(sim_data, y = DV) %>%
  binless() %>%
  vpcstats() %>%
  qpcstats()

vpc_noisy <- observed(obs_data, x = TIME, y = DV) %>%
  simulated(sim_data_noisy, y = DV) %>%
  binless() %>%
  vpcstats() %>%
  qpcstats()

base_overall <- vpc_base$qpc.stats[qpc_scope == "overall"]
noisy_overall <- vpc_noisy$qpc.stats[qpc_scope == "overall"]

cmp <- rbindlist(list(
  cbind(data.table(case = "base"), base_overall),
  cbind(data.table(case = "noisy_sim"), noisy_overall)
), fill = TRUE)

cmp_summary <- cmp[, .(
  Case = case,
  'QPC score' = qpc_score,
  'Median coverage' = coverage_penalty_med,
  'Tail coverage' = coverage_penalty_tails,
  Sharpness = sharpness_penalty,
  Interval = interval_penalty
)]]

cmp_summary[, (names(cmp_summary)[-1)] := lapply(.SD, \(x) round(x, 3)), .SDcols = names(cmp_summary)[-1]]
knitr::kable(cmp_summary, caption = "QPC summary: baseline vs noisy simulations (0 = best; lower qpc_score is better)")
```

Table 1: QPC summary: baseline vs noisy simulations (0 = best; lower `qpc_score` is better)

Case	QPC score	Median coverage	Tail coverage	Sharpness	Interval
base	0.159	0	0.092	0.272	0.391
noisy_sim	0.365	0	0.588	0.304	0.966

In this comparison you will typically see:

- **sharpness_penalty** increases with wider prediction intervals
- **interval_penalty** increases because the Winkler score increases with width (even if coverage improves)
- therefore **qpc_score** tends to increase (worse)

Compare the two plots:

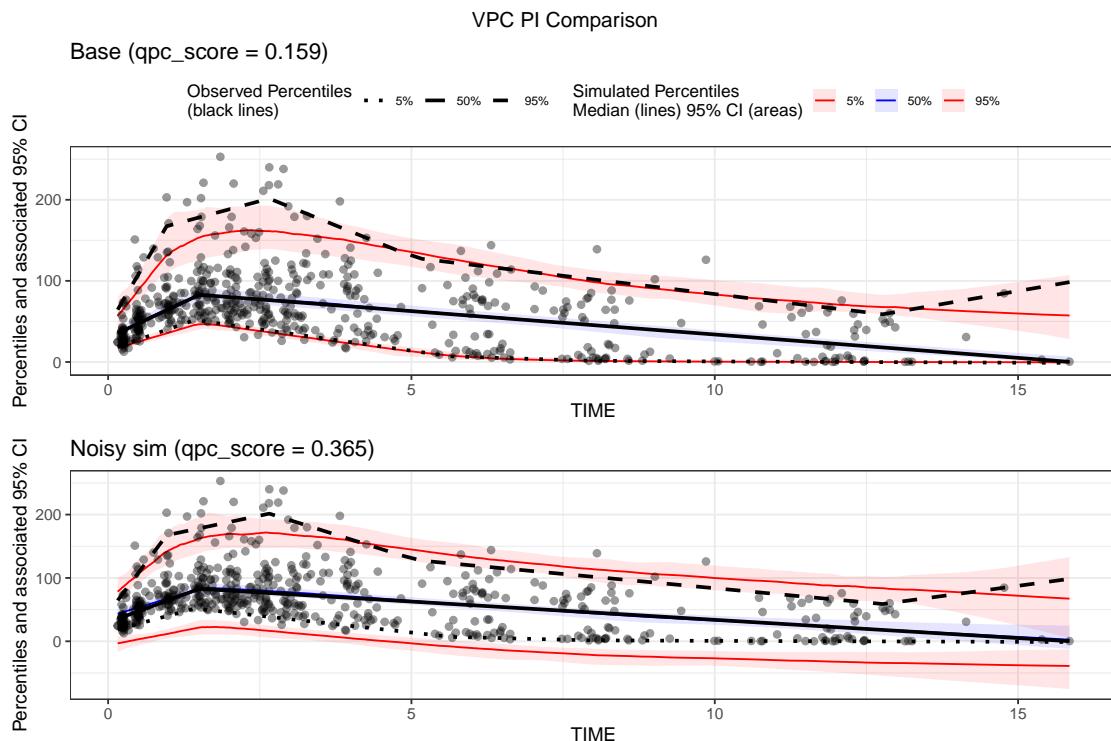
```

qpc_base <- vpc_base$qpc.stats[qpc_scope == "overall", qpc_score] [1]
qpc_noisy <- vpc_noisy$qpc.stats[qpc_scope == "overall", qpc_score] [1]

p_base <- plot(vpc_base) +
  ggplot2::ggtitle(sprintf("Base (qpc_score = %.3f)", qpc_base))

p_noisy <- plot(vpc_noisy) +
  ggplot2::theme(legend.position = "none") +
  ggplot2::ggtitle(sprintf("Noisy sim (qpc_score = %.3f)", qpc_noisy))

egg::ggarrange(p_base,
               p_noisy,
               nrow = 2, ncol = 1,
               top = "VPC PI Comparison"
)
  
```



Tips for using `sharp_ref` and `interval_ref`

By default (`sharp_ref = NULL, interval_ref = NULL`), QPC uses **self-normalizing bounded transforms** so you can score a single VPC without external calibration.

If you are comparing *many* models (e.g. search/optimization) and need more stable cross-run comparability, set:

- `sharp_ref`: a reference sharpness level (e.g. median across a model population)
- `interval_ref`: a reference interval-score level (e.g. median/75th percentile across models)

```
vpc <- qpcstats(vpc, sharp_ref = 0.15, interval_ref = 2.5)
```